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Premixed One-Dimensional Flame (PROF) Code User's Manual

Acurex Corp, Mountain View, CA Energy and Environmental Div

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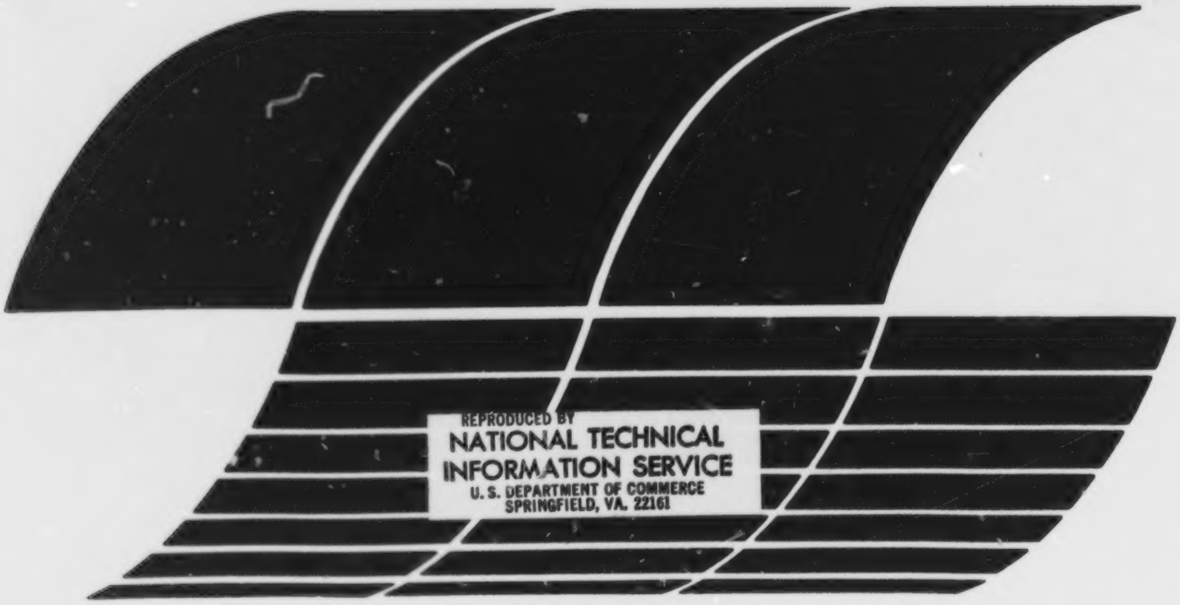

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16. ABSTRACT
The report is a user's manual that describes the problems that can be treated by the Premixed One-dimensional Flame (PROF) code. It also describes the mathematical models and solution procedures applied to these problems. Complete input instructions and a description of output are given. Several sample problem input and output listings are presented to demonstrate code options. A program listing and code Fortran variable definitions are included. The PROF code numerically models complex chemistry and diffusion processes in premixed laminar flames. Since the code includes diffusion, it gives realistic solutions of coupled combustion and pollutant formation processes in the flame zone, as well as downstream in the postflame region. The code can be a valuable aid when interpreting experimental flame data. In addition to flames, the PROF code can also treat problems involving well-stirred reactors, plug-flow reactors, and time-evolution chemical kinetics. A wide variety of conventional and experimental combustion systems can be treated by the code's flame and reactor options.

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Computer Programs	Diffusion	Stationary Sources	09B	14B
Combustion	FORTRAN	PROF Code	21B	
Flames	Mathematical	Flat Flames		
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ABSTRACT

The Premixed One-dimensional Flame (PROF) code numerically models complex chemistry and diffusion processes in premixed laminar flames. Since this code includes diffusion, it gives realistic solutions of coupled combustion and pollutant formation processes in the flame zone, as well as downstream in the post-flame region. Experience has shown that the code can be a valuable aid when interpreting experimental flame data.

In addition to flames, the PROF code can also treat problems involving well-stirred reactors, plug-flow reactors, and time-evolution chemical kinetics. A wide variety of conventional and experimental combustion systems can be treated by the code's flame and reactor options.

This PROF code user's manual describes the problems that can be treated by the code. It also describes the mathematical models and solution procedures applied to these problems. Complete input instructions and a description of output are given. Several sample problem input and output listings are presented to demonstrate code options. A program listing and code Fortran variable definitions are included in the manual.

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LIST OF SYMBOLS

A	cross sectional area
B_ν	monochromatic radiation intensity
C_j	J factor constant coefficient
C_p	specific heat
$\tilde{C}_p$	weighted specific heat defined by Equation (25)
C_w	circumference of bounding tube
CV	denotes control volume
D_{ij}	binary diffusion coefficient
$\bar{D}$	diffusion constant defined by Equation (6)
E	activation energy for kinetic reaction
F_i	diffusion factor of species i
h	enthalpy of bulk gas
i	denotes species when used as subcript
J	J factor in wall transport expression
J_i	flux of species i in axial direction

LIST OF SYMBOLS (Continued)

J_{w_i}	flux of species i at bounding tube wall
k	thermal conductivity of bulk gas
K_ν	spectral absorption coefficient
K_p	Planck mean absorption coefficient
K_{p_m}	equilibrium constant for reaction m
L	characteristic dimension of flame for radiation properties
$\dot{m}$	mass rate of gas
M	molecular weight
p	pressure
q	axial heat transport
q_w	heat transport at the bounding tube wall
Q	volumetric heat loss
q_R	radiative flux
r_w	radius of bounding tube
R	gas constant
S	distance along flame axis
S_c	Schmidt number

LIST OF SYMBOLS (Continued)

$\bar{S}$	normalized distance defined by Equation (33)
T	temperature
V	volume of well-stirred reactor or radiation integration volume
W_i	chemical production rate of species i
X_i	mole fraction of species i
Y_i	mass fraction of species i
α_i	species concentrations in moles per gram
δ	flame zone length scale
ε_g	emissivity of gas
$\nu_{i_m}^T$	third body efficiency of species i in reaction m
Ω_{ij}	integral expression which depends upon the particular intermolecular potential function which is utilized
ρ	density
σ	Stefan-Boltzmann constant
σ_{ref}	collision cross section for reference species

LIST OF SYMBOLS (Concluded)

Superscripts

P	reaction products
R	reaction reactants

SECTION 1

INTRODUCTION

This User's Manual fully describes and provides instructions for using the Premixed One-dimensional Flame (PROF) computer code.*

The PROF code can be used to predict the detailed chemical kinetic combustion and/or pollutant formation events which occur in a wide variety of experimental and practical combustion devices. Both steady, free and confined premixed flames, where gaseous diffusion is important, can be treated by the code. Also, well-stirred reactor, plug-flow reactor, and fixed mass time-evolution chemical kinetic problems, where diffusion is not explicitly treated, can be modeled by the code. References 1 and 2, as well as Section 7 of this report, present some examples of problems which can be treated by the PROF code.

The key program element in the PROF code is a stable and reliable kinetic chemistry routine. This routine can be applied to any chemical system for which kinetic reaction data is available. To model flame and reactor-type problems, appropriate driver routines are linked to the general chemistry routine. The flame model includes axial gas phase diffusion and is, mathematically, a multivariable boundary value problem. This problem requires a coupled grid solution procedure for all variables. This grid problem is solved in PROF by using a predictor - linearized corrector iterative matrix procedure. The reactor type models do not have explicit diffusion terms. These models are initial value problems solved by simple time or space marching in the PROF code.

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*Program is coded in Fortran V.

The PROF code was developed to accurately model the detailed combustion and pollutant formation processes occurring in premixed one-dimensional flames. Previous plug-flow models applied to premixed flame combustion and pollutant formation processes did not incorporate axial diffusion in the formulation. Since ignition processes require upstream diffusion, these plug-flow models could not be directly applied to flames without making some gross assumptions as to the upstream ignition zone starting conditions. In addition, the accuracy of these nondiffusive models is very poor in the flame zone, where diffusion is important. Since the PROF code includes axial diffusion, predictions of combustion and pollutant formation processes can be achieved in the flame zone as well as downstream of this zone. The accuracy of these predictions is dependent only on the adequacy of elementary kinetic reaction and transport data. Thus, PROF predictions, combined with experimental data, can provide valuable insights into the complex chemical events taking place within as well as downstream of the flame zone.

Although the PROF code was developed to treat, primarily, the premixed one-dimensional flame problem, the PROF code formulation has been expanded to include reactor-type problems which do not explicitly include axial diffusion. This single code can now be applied to a wide variety of practical and experimental combustion problems.

A brief description of the problems that can be treated by the PROF code appears in Section 2. Section 3 presents the mathematical models and boundary conditions for the flame and reactor type problems. Appropriate solution procedures for the mathematical models are given in Section 4. A full set of code input instructions are given in Section 5, and the standard output format is described in Section 6. Listings of input data and selected sections of output for several sample problems are given in

Section 7. Descriptions of debug output and a short discussion of potential problem areas appears in Section 8. Code Fortran variables and definitions are given in Section 9. Summary descriptions of the program and subroutines are presented in Section 10. A complete listing of the program appears in Section 11.

SECTION 2

PROBLEM DESCRIPTION

The PROF code is applied primarily to premixed one-dimensional laminar, laterally unconfined, flame problems. Figure 1 illustrates schematically an unconfined flame which is anchored to a flat flame burner by a flameholder. The flameholder provides a sink for the flame's "excess" heat and reactive species.

The PROF code models axial diffusion of heat, q, and species, J_i, as well as chemical kinetics within the flame. The calculations can also include radiative heat loss to the surroundings and heat and reactive species losses to the flameholder. Very general chemical systems can be treated by the code. Molecular heat and mass transport modeling incorporate accurate approximations for unequal species diffusion and nonunity Lewis number effects.

The PROF code unconfined flame option can be applied to a number of experimental and practical flame problems. For example, it can be used to analyze coupled combustion and pollutant formation processes, such as fuel-nitrogen conversion, in experimental flat flames. Also, practical problems such as determining premixed flame speeds and flamability limits of coal or oil-derived gaseous fuel mixtures can be solved with this option.

To augment the PROF unconfined flame predictive capability, models for the thermal and chemical effect of confining walls on bulk gas properties are included in the code. Figure 2 illustrates schematically the confined flame problem treated by the PROF code. In this case both axial and radial heat and mass transport are considered. Transfer coefficients are used to

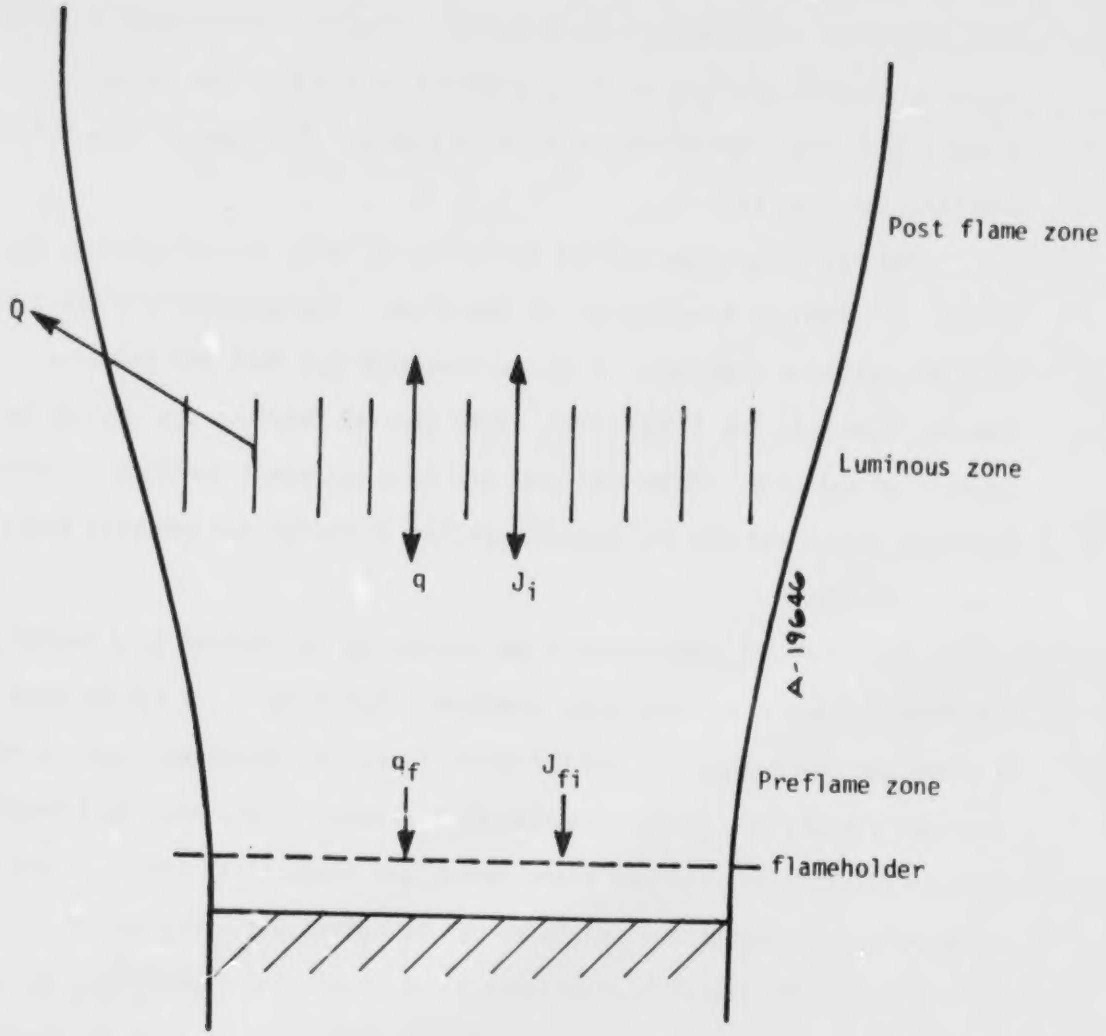


Figure 1. Schematic of unconfined flame.

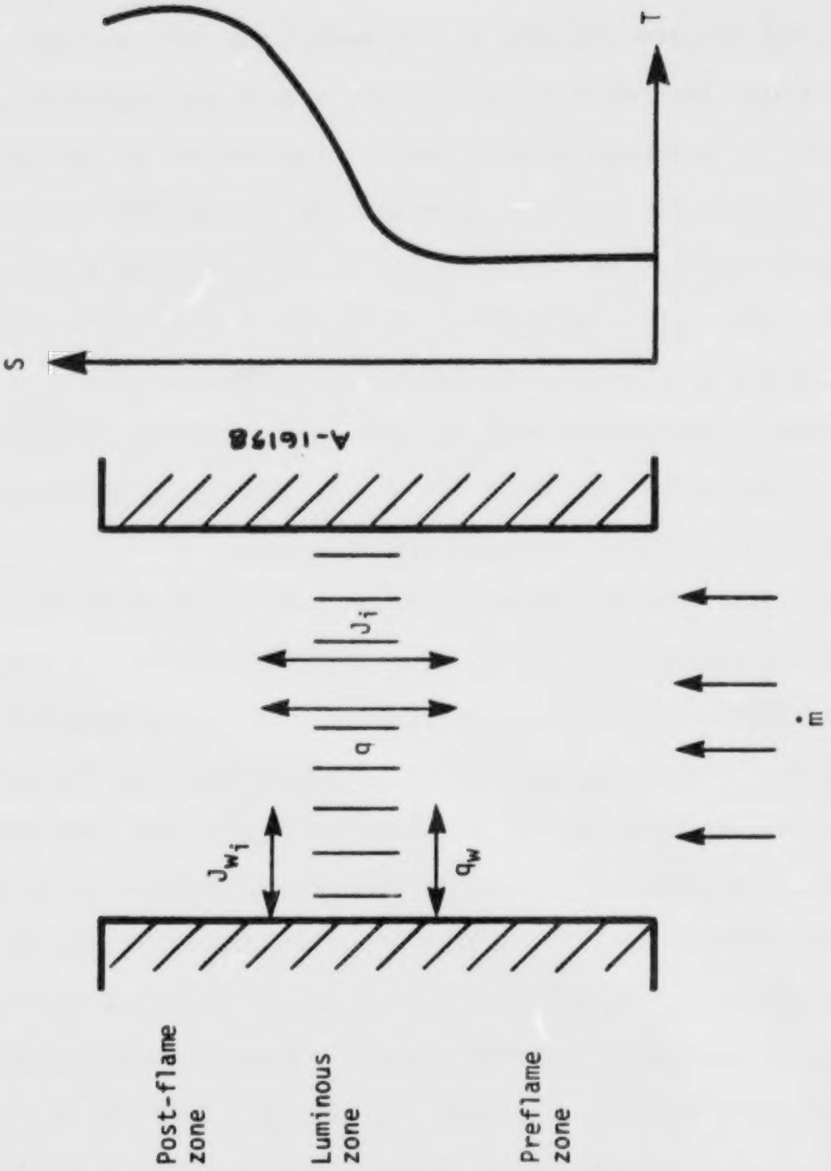


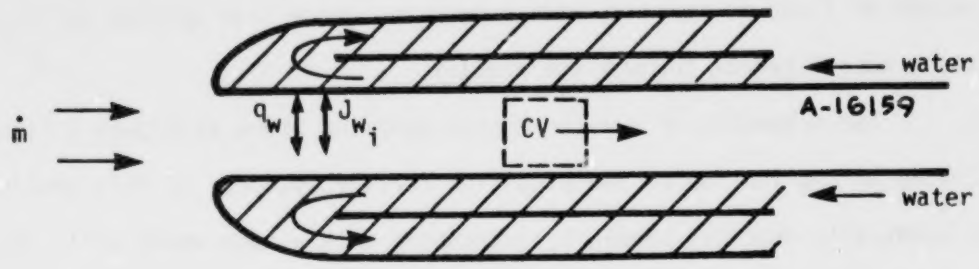
Figure 2. Schematic of confined flame.

model heat and mass tranfer to the confining walls in terms of bulk and wall gas conditions so that the efficient one-dimensional calculation scheme can be applied to this problem. The details of radial variation of composition and chemical reaction are lost in this method, but this approach is useful to assess the impact of wall effects on bulk gas properties.

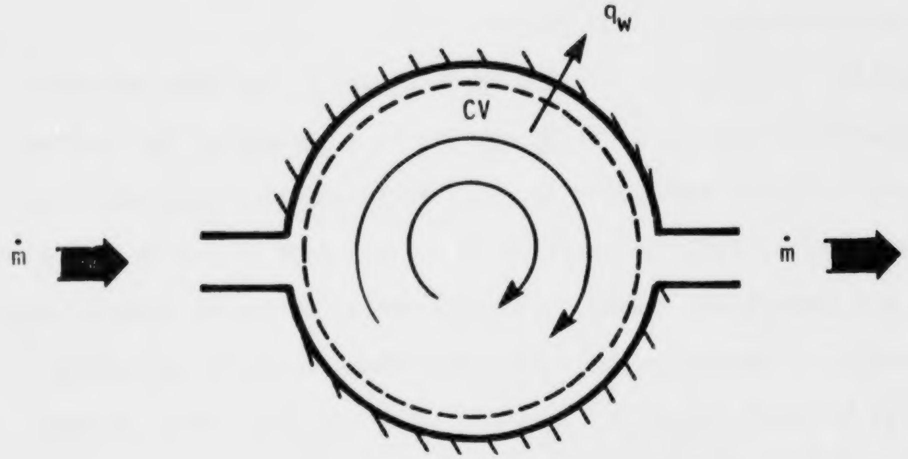
For the confined flame problem, the state of the gas at the tube wall is assigned as a boundary condition along with the initial bulk species fluxes and temperatures. The wall gases may be in equilibrium or any arbitrary kinetic state. Given the boundary conditions, the code determines bulk gas properties as a function of distance along the tube axis.

A variety of experimental and practical combustion and pollutant formation problems can be treated by this option. Some examples are tubular reactors, surface combustors, and catalytic combustors.

Besides flame problems, where axial gas phase diffusion is important, the PROF code can also treat fully-mixed, well-stirred reactor and one-dimensional nondiffusive plug-flow reactor and time-evolution chemical kinetic problems. Figure 3 illustrates schematically some possible applications of the well-stirred reactor and plug-flow reactor PROF code options. The schematic of the jet-stirred combustor illustrates an application of the well-stirred reactor option. In this problem, a specified mass of reactants and products flows continuously through a fixed-volume chamber. Intense mixing of the reactants occurs within the combustor and chemical reaction takes place uniformly throughout the chamber. Depending on the gas and wall temperatures, heat may or may not be lost through the walls



WATER-COOLED SAMPLING PROBE
(Plug-Flow Reactor)



JET-STIRRED REACTOR
(Well-Stirred Reactor)

Figure 3. Schematic of well-stirred and plug-flow reactor problems.

of the chamber. In this well-stirred reactor case a steady-state fixed volume of fluid is reacting with a mean residence time defined by the constant mass flowrate through the reactor.

The schematic of a water-cooled sampling probe in Figure 3 illustrates an application of the plug-flow reactor option. In this problem, a chemically reacting sample is introduced into a tube whose walls are cooled much below the entering gas temperature. The cooling effect of the wall quenches the gas phase reactions, allowing the sample to pass through the probe unaltered by these reactions. Besides cooling the gases, the wall might also provide sites for heterogeneous gas phase reactions which will alter the sample composition. Only radial diffusive heat and mass transfer are considered in this option.

Besides the problems illustrated in Figure 2, the plug and well-stirred reactor options can also be applied to a variety of gas turbine, furnace and catalytic combustion and pollutant formation problems. The PROF code can also treat the reaction of a fixed mass of gas in time as the pressure and temperature change. Chemical evolution inside internal combustion engines, combustion bombs and other time-dependent combustion systems can be predicted by this option. Of course the option assumes uniformly mixed and reacting mixtures within the system. Therefore, applying this option to spatially nonuniform systems represents only an approximate modeling of the system.

The following section describes the assumptions, equations and solution procedures utilized in the PROF code. The solution procedure has been optimized for predicting premixed one-dimensional flames. The following discussion will emphasize the development of the flame equations. Well-stirred and plug-flow reactor equations are subsets of the flame equations and the reduction of flame equations to these cases will be only briefly discussed.

SECTION 3

MATHEMATICAL MODELS

In this section the flame model is discussed first. This is followed by discussions of the plug-flow reactor, time-evolution chemical kinetic and well-stirred reactor models.

3.1 Flame Model

The flame option governing equations are developed by integrating the steady two-dimensional species, mass and energy equations across a plane perpendicular to the axis. This results in a set of one-dimensional flame equations in terms of bulk gas properties. These properties vary along the flame axis as a result of fluxes of heat and mass at the edge of the flame and chemical reaction and axial diffusive fluxes within the bulk gases. For a large diameter/height ratio free flame with an initially uniform flow, the edge fluxes are relatively small and the bulk properties are equivalent to local conditions across the flame. For a flame confined in a tube (e.g., catalytic combustor) the edge fluxes can be significant. In this case, the edge fluxes are approximately treated by a transfer coefficient approach where the fluxes are assumed to be directly proportional to bulk and wall gas states. Using transfer coefficients permits one-dimensional solution procedures to be applied to an essentially two-dimensional problem.

The quasi-one-dimensional flame conservation equations can be written as:

Species

$$\dot{m}\,\frac{dY_i}{ds} = AW_i - \frac{d(AJ_i)}{ds} - C_w J_{w_i} \qquad (1)$$

Energy

$$\dot{m}\frac{dh}{ds} = AQ - \frac{d}{ds}\left(\sum_i AJ_ih_i + Ak\frac{dT}{ds}\right) - C_wq_w \tag{2}$$

where global continuity has been incorporated into the above equations. The momentum equation has been replaced by assigning pressure. Assigning a fixed pressure is a valid approximation for the low-velocity flame cases of primary interest. The species conservation expression, Equation (1), shows that the species mass fraction along the flame axis is altered by species bulk gas phase chemical production, W_i, axial diffusive flux, J_i, and wall diffusive flux, J_{w_i}. In the energy conservation expression, Equation (2), the enthalpy along the flame axis is altered by the bulk gas heat loss rate, Q, axial diffusive heat flux, $\sum_i J_ih_i + k\, dT/ds$, and wall heat loss, q_w. Expressions for W_i, J_i, J_{w_i}, Q, K and q_w, along with boundary conditions, complete the definition of the flame problem.

3.1.1 Species Axial Diffusional Flux

Utilizing binary coefficient data, the rigorous expression for species multicomponent diffusional flux can be obtained by implicitly solving the Stefan-Maxwell relations. This involves a level of effort which, in most practical flame cases, is beyond that consistent with the quality of the transport data input into the code. For the PROF code the simple, yet adequate, bifurcation approximation for the binary diffusion coefficients is used with the Stefan-Maxwell relations to develop an explicit expression for species flux.

The approximation, which is fully developed in Reference 3 and summarized in Appendix A,assumes that the contributions of species i and j to the diffusion coefficients, $\mathcal{D}_{ij}$, can be separated in the following manner:

$$\mathcal{D}_{ij} = \frac{\overline{D}}{F_i F_j} \tag{3}$$

where $\overline{D}$ is a reference self-diffusion coefficient and F_i and F_j are diffusion factors. For binary and ternary systems, Equation (3) is exact. The pressure and temperature dependence of $\mathcal{D}_{ij}$ is absorbed into $\overline{D}$ so that F_i and F_j are independent of temperature and pressure. For more complex systems, equation (3) may be considered as a good correlating function of diffusion data. The primary advantage of this approximation is that it permits an explicit formulation for diffusional mass flux J_i in terms of gradients of species i to be developed from the Stefan-Maxwell relations. Neglecting thermal diffusion effects, the flux can be written in the following form (see Appendix A):

$$J_i = -\frac{\rho\overline{D}}{\mu_1 F_i}\left(\frac{dY_i}{ds} + \left(\frac{Y_i}{M}\right)\left(\frac{dM}{ds} - F_i\frac{d\mu_2}{ds}\right)\right) \tag{4}$$

where

$$\mu_2 = M\sum Y_i/F_i \quad \text{and} \quad \mu_1 = \sum X_i F_i \tag{5}$$

where Xi and Yi are the mole and mass fractions, respectively. Computations that consider this formulation are considerably more efficient than those that use arbitrary expressions for the $\mathcal{D}_{ij}$ and apply either the Stefan-Maxwell implicit equations or develop the concentration dependent multicomponent diffusion coefficients.

In Equation (4), $\overline{D}$ is typically taken as the self-diffusion coefficient of some reference species, e.g., O_2. The F_i are taken as constants independent of temperature and pressure. From Reference 4:

$$\overline{D} = 2.628 \times 10^{-3} \frac{T(T/M_{ref})^{1/2}}{P\sigma^2_{ref}\Omega^{(1,1)*}_{ij}} \quad (\text{cm}^2/\text{sec}) \tag{6}$$

with T in °K, P in atmospheres, and collision cross section, σ in Å. For O_2 as the reference species, σ is equal to 3.467 Å. From Appendix A the integral expression for transport properties is approximated by:

$$\Omega^{(1,1)*}_{ij} \approx 1.07\ [T/(\varepsilon/k)]^{-0.159} \tag{7}$$

where the maximum energy of attraction function, ε/k, for O_2 is 106.7 and thus:

$$\begin{aligned} \overline{D} &= 0.172 \times 10^{-4}\ T^{1.659}/P \quad (\text{cm}^2/\text{sec}) \\ &= \tilde{D}\ T^{1.659} \end{aligned} \tag{8}$$

Introducing Equation (8) into Equation (4) gives the axial species diffusional flux expression:

$$J_i = - \frac{PM\tilde{D}T^{0.659}}{\mu_1 R\, F_i} \left(\frac{dY_i}{ds} + \left(\frac{Y_i}{M}\right)\left(\frac{dM}{ds} - F_i \frac{d\mu_2}{ds}\right)\right) \tag{9}$$

3.1.2 Species Production Terms

Each W_i in the species conservation equation represents a summation of contributions from all reactions which include that species. For reactions of the type:

$$\sum_i \mu_{i_m}^R B_i \rightleftarrows \sum_i \mu_{i_m}^P B_i$$

where μ are the stoichiometric coefficients on species B_i. W_i can be written as:

$$W_i = M_i \sum_m \left(\mu_{i_m}^P - \mu_{i_m}^R\right) R_m \tag{10}$$

where

$$R_m = k_{f_m} \left[e^{\Sigma\mu_{i_m}^R \ln p_i} - e^{\Sigma\mu_{i_m}^P \ln p_i - \ln K_{p_m}}\right] \times \sum_i \nu_{i_m}^T p_i \tag{11}$$

and $\nu_{i_m}^T$ denotes third body efficiency of species i. The forward reaction rate coefficient, k_{f_m}, has the Arrhenius form:

$$k_{f_m} = aT^b e^{-(E/RT)} \tag{12}$$

The backward reaction rate coefficient is taken to be equal to the forward reaction rate coefficient divided by the equilibrium constant.

As discussed in detail in Reference 5 the solution of these equations is subject to several pitfalls which need to be carefully circumvented. The most discussed problem is associated with k_{f_m} becoming very large, forcing the bracketed term in Equation (11) to zero to maintain a finite net contribution of the term to the species conservation equation. Forcing the bracketed term toward zero is equivalent to imposing equilibrium. Because the term appears in several species equations, it is necessary to combine these equations in such a way that this equilibrium relation effectively replaces only one mass balance relation.

Even with the rearrangement of equations, the iterative Newton-Raphson procedure used to solve the simultaneous equation set can be defeated if a significant change has occurred in the character of the equations. In the PROF chemical kinetics package a combination of gradual recharacterization of equations and damping has proved highly successful in determining a solution. This is very important if an efficient grid-type coupled diffusion/kinetics boundary value solution is to be achieved.

3.1.3 Species Flux at the Wall

For a flame situated in a bounding tube with reactive walls, a net species flux to the wall develops which is rigorously a function of the detailed radial distribution of species concentration at the wall. For efficient computations, the PROF formulation utilizes a transfer coefficient approach to establish the species flux at the wall. In this approach, the species flux is assumed to be directly proportional to the difference between the bulk and wall gas composition. Since it is not necessary to know the detailed radial species concentration distribution, this formulation allows an efficient axial-direction, one-dimensional computational scheme to be retained. For consistency, the wall flux proportionality factor is developed in a manner similar to the axial species diffusion case. Analogous to the axial diffusion expression, the wall species flux is written as:

$$J_{w_i} = \rho u\,[J] \cdot Sc^{-n}\,\frac{1}{\mu_1 F_i}\left(Y_i - Y_{w_i}\right) \tag{13}$$

with the J factor being represented by a simple Reynold's number relation, $C_J \cdot Re^{-m}$. The Schmidt number, $\mu/\rho\overline{D}$, adjusts the J factor to a transfer coefficient appropriate to the reference species; the $\mu_1 F_i$ corrects it further for the specific species in question. Consistent with the accuracy of typical J-factor correlations (see Reference 6) the molecular weight and μ_2 gradients (as in Equation 9) have been neglected in the driving potential formulation.

3.1.4 Bulk Gas Volumetric Heat Loss

The term Q in the energy equation is a bulk gas phase volumetric heat source, or sink term. If desired, Q can be assigned as a constant or as a function of distance along the flame axis. However, most often Q, for unconfined flames, is the volumetric heat loss due to radiation. The PROF code formulation includes logic to model heat loss due to radiation for nonsooting flames.

The radiation heat loss, is written as:

$$\int_S QA\,ds = -\int_V (\vec{\nabla} \cdot \vec{q})\,dV \tag{14}$$

where $\vec{\nabla} \cdot \vec{q}$ is the divergence of the radiative flux. For conditions where the flame radius is small compared to all absorption coefficients at all frequencies (i.e., $\int_0^{r_w} K_\nu \, dr \ll 1$ for all ν), and where radiation back from the environment can be neglected, Q_r becomes (Reference 7):

$$Q_r = -4K_p \sigma T^4 \tag{15}$$

where K_p is the Planck mean absorption coefficient given by:

$$K_p = \frac{\pi}{\sigma T^4} \int_0^\infty K_\nu B_\nu \, d_\nu \tag{16}$$

This is the emission-dominated or optically thin limit approximation which is valid for typical nonsooting laboratory flames. To complete the definition of radiative heat loss, K_p values are now defined.

The major radiating species in hydrocarbon flames are CO_2, H_2O, and CO. For each of these species, there are roughly one to four important radiation bands scattered through the 1 to 15 micron wavelength range of interest.* Each band typically occupies a relatively narrow region of the spectrum and can be separated from adjacent bands by a region which neither absorbs nor emits thermal radiation. The properties of the band systems are required to properly calculate emission losses.

Rigorously, the spectral absorption coefficient, K_ν, is available only for the individual line spectra and applying this property requires much effort. Therefore, its usefulness is limited in applications requiring just heat loss from combustion products. An alternate (and simpler) approach is to use a wide band absorption model. In the PROF code the wide band model correlation parameters of Edwards and Balakrishnan (Reference 9) are utilized to determine the emissivity of CO_2, H_2O, and CO. The Planck mean absorption coefficient is determined from the gas emissivity by using the optically thin limit expression (Reference 10):

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*Approximately 2 to 20 percent of the energy released in combustion becomes infrared radiation, whereas only 0.4 percent becomes visible or ultraviolet radiation (Reference 8). Therefore, only infrared radiation need be considered.

$$K_p = \frac{1}{2} \frac{\varepsilon_g}{L} \bigg|_{L \to o}$$

where ε_g is the gas emissivity and L is the characteristic dimension of the system. Calculated Planck mean absorption coefficients for temperatures between 400°K and 2600°K are given in Figure 4 for the pure gaseous components CO_2, H_2O and CO at a total pressure of 1 atm. For all cases, the path length, L, is taken as 0.001 feet, a number which is small enough to ensure recovery of optically thin data. As shown, CO_2 is a strong radiator at high temperatures compared to H_2O and CO. The emissivities, from which the K_p values were obtained, have been compared to available data (Reference 11). For an assumed pressure-pathlength product of 0.01 atm-foot at a total pressure of 1 atm, the calculated results were within 10 percent of the reported data. This agreement lends confidence to the use of the K_p's given in Figure 4.

To establish K_p for a mixture of gases at any pressure, a simple summation scheme was derived which considers radiatively noninteracting gases. This expression has the form:

$$K_p = P \sum_i X_i K_{p_i} \qquad (17)$$

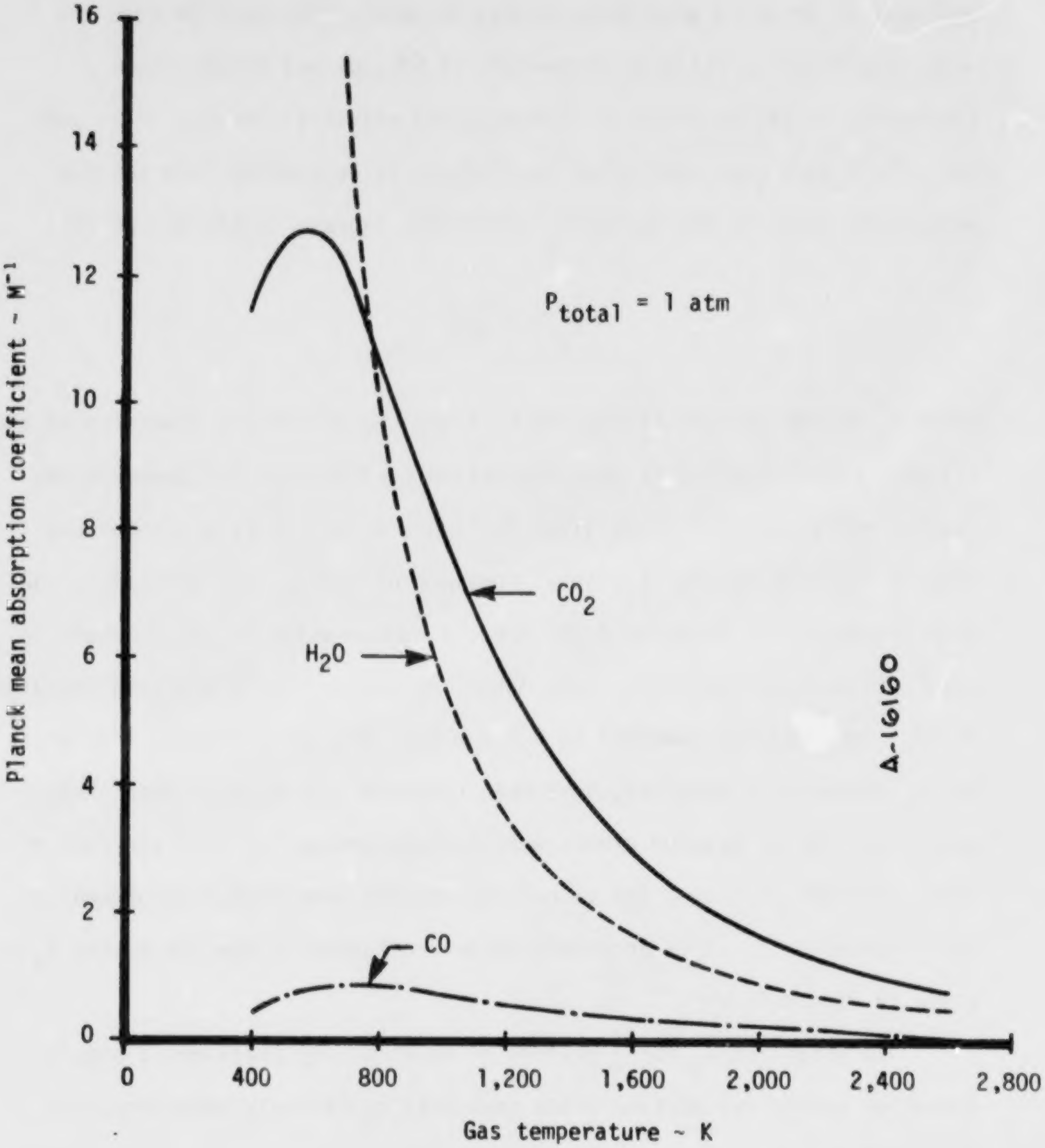


Figure 4. Planck mean absorption coefficients at one atmosphere total pressure.

and is valid as long as the optically thin approximation is valid. Applying data given in Figure 4, Equation (17) and the heat loss relationship, Equation (15), the radiation heat loss in flames is established.

3.1.5 Axial Diffusional Heat Flux

The axial diffusional heat flux consists of a species enthalpy transport term, $A\sum_i J_i h_i$, and a conduction transport term, AkdT/ds. The species flux J_i has been defined in Section 3.1.1. To fully define the axial diffusional heat flux, an expression for mixture thermal conductivity, k, must be developed.

As mentioned previously, accurate multicomponent transport properties for all flame conditions are not available and approximations are in order to provide simple, yet adequate, transport coefficient data for practical flame calculations. In this spirit, the code thermal conductivity expression is developed from approximate relationships and some diffusion factor concepts which were used in Section 3.1.1.

The thermal conductivity of a mixture of polyatomic molecules can be written (Reference 4) as:

$$k_{mix} = k_{mono\text{-}mix} + k_{int} \tag{18}$$

where $k_{mono\text{-}mix}$ is the mixture thermal conductivity computed neglecting all internal energy modes and k_{int} is the contribution of the internal energy modes of the molecules to the mixture conductivity. An approximate relationship for $k_{mono\text{-}mix}$ developed by Mason and Saxena (Reference 12) is:

$$k_{mono\text{-}mix} = \sum_{i}^{I} \left[\frac{X_i k_{i_{mono}}}{X_i + 1.385 \frac{RT\mu_i}{PM_i} \sum_{j \neq 1}^{I} \frac{X_i}{\mathcal{D}_{ij}}} \right] \tag{19}$$

where $k_{i_{mono}}$ is the thermal conductivity of the pure species i, neglecting all internal degrees of freedom, and μ_i is the viscosity of species i. Expressions for $k_{i_{mono}}$ and μ_i can be written (Reference 4) as:

$$k_{i_{mono}} = \frac{15}{4} \frac{R}{M_i} \mu_i \tag{20}$$

$$\mu_i = \frac{5}{6A^*_{ii}} \rho_i \mathcal{D}_{ii} \tag{21}$$

where A^*_{ii} is a ratio of collision integrals. Based on a Lennard-Jones intermolecular potential the value of this parameter will be between 1.10 and 1.14. A value of 1.12 has been chosen here and the 1.385 adjusted to 1.344* to allow the elimination of additional terms. Introducing $k_{i_{mono}}$ and μ_i, Equations (20) and (21), respectively, and $\mathcal{D}_{ij}$, defined in Equation (3), into Equation (19) the expression for $k_{mono\text{-}mix}$ becomes:

$$k_{mono\text{-}mix} = \frac{\rho\bar{D}}{\mu_1} \left\{ \sum \left[\frac{\frac{X_i}{F_i} \frac{15}{4} \frac{R}{M}}{1.344} \right] \right\} \tag{22}$$

To complete the definition of k, the expression for the internal energy mode contribution to thermal conductivity must be added to Equation (22).

*A value of 1.385 x 1.065 was actually used in Reference 4, but subsequent papers co-authored by Mason dropped the 1.065.

From Equations (59) and (77) of Reference 13, the following relation can be obtained:

$$K_{int} = \sum_i \frac{\rho X_i \frac{M_i}{M} \left(C_{pi} - \frac{5}{2} \frac{R}{M_i}\right)}{\sum_j x_j / \mathcal{D}_{ij}}$$

which with Equations (3) and (5) yields:

$$k_{int} = \sum \frac{\rho \bar{D} X_i \frac{M_i}{M} \left(C_{p_i} - \frac{5}{2} \frac{R}{M_i}\right)}{\mu_1 F_i} \tag{23}$$

The value of k used in PROF is then:

$$k = \frac{\rho \bar{D}}{\mu_1} \left\{ \tilde{C}_p + 0.29\ R\ \mu_3 \right\} \tag{24}$$

where

$$\mu_3 = \frac{1}{M} \sum_i \frac{X_i}{F_i} \quad \text{and} \quad \tilde{C}_p = \frac{1}{M} \sum \frac{M_i X_i C_{p_i}}{F_i} \tag{25}$$

3.1.6 Wall Heat Flux

A flame situated in a nonreactive tube at a fixed wall temperature will either lose or gain heat through the wall depending on the bulk gas temperature. If the wall is reactive, then an additional heat loss or gain comes into play depending on wall and bulk gas composition. As in the wall species flux, the PROF code formulation treats the wall heat flux by assuming that, for the nonreactive wall case, heat flux is proportional to the difference between bulk and wall gas temperatures. For the reactive wall case, a more general expression is used to account for the heat released by chemical reactions which occur between the bulk gas and wall. The completely general expression for wall heat flux is then:

$$q_w = \rho u \, [J] \, Sc^{-n} \, \frac{1}{\mu_1} \left[\tilde{h} - \tilde{h}_w + \left(\frac{k\mu_1}{\rho\bar{D}} - \tilde{C}_p \right) \left(T - T_w \right) \right] \tag{26}$$

where, again, the J factor introduced in Equation (13) is used. With $\tilde{h}$ defined by:

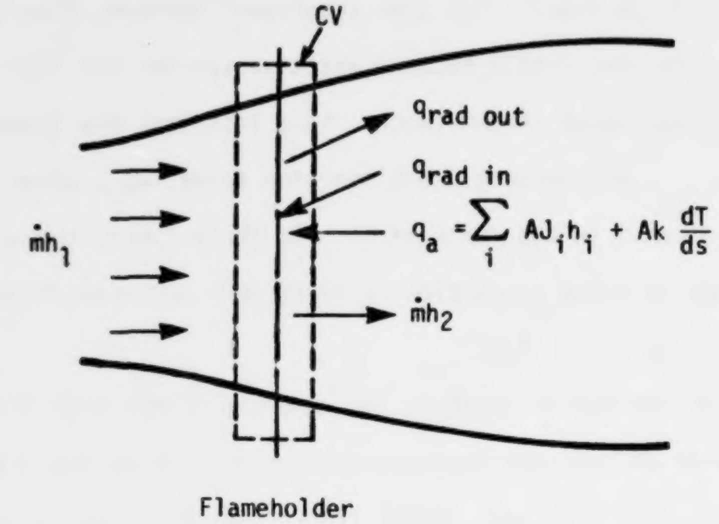
$$\tilde{h} \equiv \frac{1}{M} \sum \frac{M_i X_i H_i}{F_i} \tag{27}$$

It is noted that the driving potential reduces to the temperature difference for constant composition.

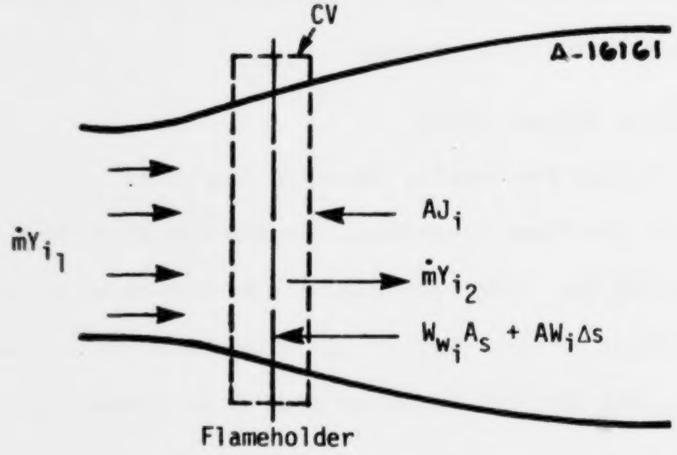
3.1.7 Specialized Boundary Conditions

For flames propagating in free space, the upstream boundary conditions are the unburnt gas temperature and composition and the downstream boundary condition is that of negligible diffusion of species and heat. In the laboratory, flames are typically anchored to their burners by the use of flameholder grids. These grids stabilize the flame by providing a sink for the flames "excess" heat or reactive species. While stabilizing the flame, these grids also alter the flame properties from those that would be achieved in free space. For accurate prediction of laboratory burner flames, the effects of flameholder processes on flame properties must be included in the code modeling.

Figure 5 illustrates schematically the heat and species balances which develop around a flameholder grid. Of primary importance is the absence of heat or reactive species diffusion upstream of the grid. The amounts of heat or reactive species which diffuse from the downstream region to the flameholder grid depend on the ratio of burner flow speed to



Heat Balance at Flameholder



Mass Balance at Flameholder

Figure 5. Schematic of flameholder processes.

free space flame speed. For some laboratory burners, flow speeds are adjusted such that little heat or reactive species are lost to the flameholder. Under these circumstances, heat loss from the flameholder, terms $-q_{r_{in}} + q_{r_{out}}$, and heterogeneous reaction terms, W_{w_i}, shown in Figure 5, may be neglected in the formulation. In these cases, the only effect of the flameholder on flame properties is to prevent upstream diffusion of heat or species to the burner face.

When the burner speed is low compared to the free flame speed, significant amounts of heat and reactive species diffuse to the flameholder. For these cases, the PROF code models flameholder heat loss by assigning a fixed temperature to the gas at the flameholder. In addition to the heat loss, heterogeneous recombination of reactive species which diffuse to the flameholder are modeled by locally increasing the homogeneous recombination reaction rates to very high values.

3.2 Plug-Flow Reactor Model

As indicated previously, the plug-flow reactor conservation equations are subsets of the flame equations. The primary difference between the plug-flow reactor and the flame equations is the absence of axial diffusion effects for the plug-flow reactor. Deleting axial diffusion terms from Equations (1) and (2), the plug-flow reactor equations are:

Species

$$\dot{m} \frac{dY_i}{ds} = AW_i - C_w J_{w_i} \tag{28}$$

Energy

$$\dot{m} \frac{dh}{ds} = AQ - C_w q_w \tag{29}$$

The expressions for W_i, J_{w_i}, Q and q_w remain the same as in the flame case (see Sections 3.1.2, 3.1.3, 3.1.4 and 3.1.5). Since axial diffusion is not present, only upstream and wall composition and temperature values are needed as boundary conditions.

3.3 Time-Evolution Chemistry Problem

For the reaction of a fixed mass of gas in time as the pressure and temperature change, Equation (28) must be reinterpreted. Dropping wall effects, Jw_i, and combining ds, $\dot{m}$ and A, Equation (28) becomes:

Species

$$dY_i = \left(\frac{Ads}{\dot{m}}\right) W_i \tag{30}$$

For the time-dependent problems, the parameter $(Ads/\dot{m})$ is now interpreted as a time differential divided by the density of the fixed mass of the gas, or:

$$\frac{dt}{\rho} \equiv \frac{Ads}{\dot{m}}$$

Only the initial mixture composition and assigned pressure and temperature are needed as boundary conditions for this problem.

3.4 Well-Stirred Reactor Model

The well-stirred reactor problem is different from the flame case in several respects. In a well-stirred reactor, gas composition and temperature are assumed to be uniform in both time and space within the reactor. The spatial uniformity is a result of intense mixing and the time uniformity is due to the specification of steady and equal mass fluxes into and out of the reactor. Unlike the flame and plug-flow reactor cases, algebraic equations rather than differential equations define the well-stirred reactor problem These equations can be written:

Species

$$Y_{out} - Y_{in} = \frac{V}{\dot{m}} W_i \qquad (31)$$

Energy

$$h_{out} - h_{in} = \frac{V}{\dot{m}} Q \qquad (32)$$

where V is the reactor volume and all other quantities are the same as those defined in Equations (1) and (2). If reactor volume is associated with the product, A ds and differentials replace the differences in Equations (30) and (31), then the well-stirred reactor problem is seen to be equivalent to a single step in the plug-flow reactor problem. Since the solution "time step", $V/\dot{m}$, is typically very large in well-stirred reactor problems, it is essential that a stable and reliable kinetic chemistry solver be employed. Fortunately, the chemistry solver developed for predicting flame problems is ideally suited for solving well-stirred reactor problems.

The boundary conditions applied in the well-stirred reactor case are the assignment of inlet species concentrations and enthalpy.

SECTION 4

SOLUTION PROCEDURES

The solution procedures adopted for the treatment of the set of equations developed in Section 3 are presented in this section. The highly coupled nature of the equations requires a careful solution formulation if an efficient and reliable procedure is to be realized. The principal focus of this section is on the various aspects of the flame solution procedure with lesser emphasis on the plug-flow and well-stirred reactor solution procedures.

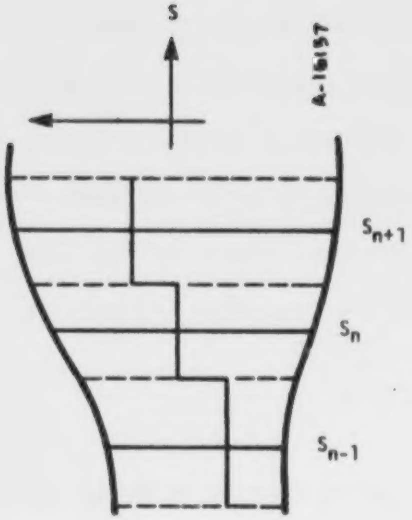
4.1 Flame Solution Procedure

The flame solution procedure is treated in three subsections. The first describes the finite difference treatment of the conservation equations, the second the chemistry solution procedure and the third the linearized predictor-corrector iteration-scheme for the overall solution.

4.1.1 Finite Difference Form of the Flame Conservation Equations

The governing differential equations (Equations (1) and (2)) are cast into algebraic form by applying simple linear finite differences. The resulting set of algebraic equations are then solved utilizing matrix procedures.

The following schematic illustrates the control volumes from which the finite difference forms of the equations are developed.



Constant properties assumed in control volumes bounded by

$$\frac{S_n + S_{n+1}}{2} \text{ and } \frac{S_{n-1} + S_n}{2} \text{ , etc.}$$

Introducing the normalized distance coordinate $\overline{s}$ defined by:

$$d\bar{s} = \frac{A_o ds}{A\rho T^{1.659}} \tag{33}$$

and applying simple linear finite differencing, the species equation becomes:

Species

$$\begin{aligned} Y_{i_n} - Y_{i_{n-1}} = {} & \left[\frac{A^2 W_i \rho T^{1.659}}{\dot{m}}\right]_n \left(\frac{\overline{S}_{n+1} - \overline{S}_{n-1}}{2}\right) + \frac{\tilde{D}}{\dot{m}F_i}\left[\frac{2}{\mu_{1_{n+1}} + \mu_{1_n}}\left(\frac{Y_{i_{n+1}} - Y_{i_n}}{\overline{S}_{n+1} - \overline{S}_n}\right)\right. \\ & - \frac{2}{\mu_{1_n} + \mu_{1_{n-1}}}\left(\frac{Y_{i_n} - Y_{i_{n-1}}}{\overline{S}_n - \overline{S}_{n-1}}\right) - Y_{i_n}\left\{\frac{1}{\mu_{1_{n+1}} + \mu_{1_n}}\left(\frac{1}{\overline{S}_{n+1} - \overline{S}_n}\right)\left(M_{n,n+1}\right.\right. \\ & \left.\left. + F_i \mu_{n+1,n}\right) + \frac{1}{\mu_{1_n} + \mu_{1_{n-1}}}\left(\frac{1}{\overline{S}_n - \overline{S}_{n-1}}\right)\left(M_{n,n-1} + F_i \mu_{n-1,n}\right)\right\} \end{aligned}$$

$$+ Y_{i_{n+1}} \left\{ \frac{1}{\mu_{1_{n+1}} + \mu_{1_n}} \left(\frac{1}{\bar{S}_{n+1} - \bar{S}_n} \right) \left(M_{n+1,n} + F_i \mu_{n,n+1} \right) \right\}$$

$$+ Y_{i_{n-1}} \left\{ \frac{1}{\mu_{1_{n-1}} + \mu_{1_n}} \left(\frac{1}{\bar{S}_n - \bar{S}_{n-1}} \right) \left(M_{n-1,n} + F_i \mu_{n,n-1} \right) \right\} \qquad (34)$$

$$- \frac{C_w}{\dot{m}} \quad \frac{S_{n+1} - S_{n-1}}{2} \quad \frac{A \rho T^{1.659}}{A_o} \quad J_{w_i}$$

where

$$M_{ij} = \frac{M_i - M_j}{M_j} \text{ and } \mu_{ij} = \frac{\mu_{2_i} - \mu_{2_j}}{M_j} \qquad (35)$$

Dividing through by molecular weight, M_i, and utilizing the composite quantities:

$$a_n = \frac{A_n^2 \delta}{\dot{m} A_o} = APR \left(\frac{A_n}{A_o}\right)^2$$

$$b_i = \frac{\tilde{D} A_o}{\dot{m} \delta F_i} = \frac{BP}{F_i} \tag{36}$$

$$\sigma_n = \frac{\overline{S}_{n+1} - \overline{S}_n}{\delta} = DS_n$$

the final form of the species equation is given by:

$$\begin{aligned}
\alpha_{i_n} - \alpha_{i_n} - \left[PM\ a\ \frac{T}{R}^{0.659}\ r_i\right]_n \left(\frac{\sigma_{n-1} + \sigma_n}{2}\right) = b_i \Bigg[& \frac{2}{\mu_{1_{n+1}} + \mu_{1_n}} \left(\frac{\alpha_{i_{n+1}} - \alpha_{i_n}}{\sigma_n}\right) \\
& - \frac{2}{\mu_{1_n} + \mu_{1_{n-1}}} \left(\frac{\alpha_{i_n} - \alpha_{i_{n-1}}}{\sigma_{n-1}}\right) - \alpha_{i_n} \Bigg\{ \left(\frac{1}{\mu_{1_{n+1}} + \mu_{1_n}}\right) \frac{1}{\sigma_n} \left(M_{n,n+1} + F_i\, \mu_{n+1,n}\right) \\
& + \left(\frac{1}{\mu_{i_n} + \mu_{1_{n-1}}}\right) \frac{1}{\sigma_{n-1}} \left(M_{n,n-1} + F_i\, \mu_{n-1,n}\right) \Bigg\} \\
& + \alpha_{i_{n+1}} \left(\frac{1}{\mu_{1_{n+1}} + \mu_{1_n}}\right) \frac{1}{\sigma_n} \left(M_{n+1,n} + F_i\, \mu_{n,n+1}\right)
\end{aligned} \tag{37}$$

$$+ \alpha_{i_{n-1}} \left(\frac{1}{\mu_{1_{n-1}} + \mu_{1_n}}\right) \frac{1}{\sigma_{n-1}} \left(M_{n-1,n} + F_i \mu_{n,n-1}\right) \qquad (37)$$

$$- \frac{C_w \delta}{\dot{m}} \frac{\sigma_n + \sigma_{n-1}}{2} \frac{A}{A_o} \rho T^{1.659} \frac{J_{w_i}}{M_i}$$

The energy equation is developed in a similar manner and leads to

$$h_n - h_{n-1} = \frac{2b_p/\sigma_n}{\mu_{1_{n+1}} + \mu_{1_n}} \left[\tilde{h}_{n+1} \left(1 + M_{n+1,n}\right) - \tilde{h}_n \left(1 + M_{n,n+1}\right)\right.$$

$$\left. + h_{n+1} \mu_{n,n+1} - h_n \mu_{n+1,n} + \chi_n \left(T_{n+1} - T_n\right)\right]$$

$$- \frac{2b_p/\sigma_{n-1}}{\mu_{1_n} + \mu_{1_{n-1}}} \left[\tilde{h}_n \left(1 + M_{n,n-1}\right) - \tilde{h}_{n-1} \left(1 + M_{n-1,n}\right)\right. \qquad (38)$$

$$\left. + h_n \mu_{n-1,n} - h_{n-1} \mu_{n,n-1} + \chi_{n-1} \left(T_n - T_{n-1}\right)\right]$$

$$- \frac{\delta}{\dot{m}} \frac{\sigma_n + \sigma_{n-1}}{2} \frac{A}{A_o} \rho T^{1.659} \left[C_w q_w + AQ\right]$$

where

$$\chi_n = \left\langle \frac{k\mu}{pD} - \tilde{C}_p \right\rangle_{n,\, n+1} - \frac{1}{2} \left(\tilde{C}_{p_{n+1}} M_{n+1,n} + C_{p_{n+1}} \mu_{n,n+1}\right.$$

$$\left. + \tilde{C}_{p_n} M_{n,n+1} + C_{p_n} \mu_{n+1,n}\right)$$

If guesses are inserted into Equations 37 and 38 for α_i, T, $\tilde{h}$ and h at the downstream station, n + 1, the equations can then be rearranged to give the unknown variables α_i, T and h at station n in terms of the guessed downstream variables, the known upstream variables, wall species and heat loss, and chemical production, W_i, at station n. The chemistry solution procedure used to determine α_i, T and h at station n, including the chemical production term W_{in}, is the key program element in the PROF code.

4.1.2 Chemistry Solution Procedure

For accuracy and numerical stability a fully implicit chemical kinetic solution procedure is employed in PROF. In this method the production rate of each reaction is a function of species concentrations at the grid location being calculated. This results in a nonlinear system of simultaneous equations for all the unknown species concentrations plus temperature. These equations are solved by inputting first guesses into the equations and then using a Newton-Raphson iterative solution procedure to correct these guesses.

The Newton-Raphson procedure, as applied in the PROF code can be summarized by considering a set of equations of the general form:

$$g_j\left(V_1, V_2 \dots V_n\right) = 0 \tag{39}$$

During the solution procedure there exists a set of estimates, V_i, for all the variables which will typically not satisfy Equation (39) and thereby will give a non-zero g_j value, or error, ε_j. The Newton-Raphson method "drives" these errors toward zero by evaluating the change in each unknown variable, ΔV_i, which would reduce the errors in all equations to zero if the functions, g_j, were linear. The correction to V_i needed to drive ε_j to zero is based on the current values of the unknown variables and the corresponding array of values of the partial derivatives $\partial g_j/\partial V_i$. This can be written as:

$$dg_j = \sum_i \frac{\partial g_j}{\partial v_i} dv_i \tag{40}$$

This relation can be inverted to yield

$$dv_i = \sum_j \left(\frac{\partial g_i}{\partial v_j} \right)^{-1} dg_j$$

which when integrated, presuming the partial derivatives constant, yields

$$\Delta v_i = \sum_j \left(\frac{\partial g_i}{\partial v_j} \right)^{-1} \Delta g_j \tag{41}$$

But Δg_j represents the desired change in g_j which is simply $-g_j$. Successive iterations, if properly constrained and/or linearized, will drive g_j to zero. In the PROF code chemistry solution, the partial derivatives use the variables, ℓnP_i, ℓnT and ℓnPM and (41) yields, for example:

$$d(\ell nP_i) = \sum_j \frac{\partial \ell nP_i}{\partial g_j} dg_j \tag{42}$$

which if taken as linear all the way to solution gives:

$$\left(\Delta \ln P_i\right) \approx \sum_j \left(\frac{\partial \ln P_i}{\partial g_j}\right) \left(-g_j\right) \tag{43}$$

When the initial guesses, V_i, are close to the solution and the equations are fairly linear, the straightforward application of the above Newton-Raphson iterative solution procedure is rarely defeated. With substantial chemical kinetics neither of these two conditions can be expected and achieving a solution by straightforward application of the method is not assured. In the PROF code a procedure has been implemented which has greatly increased the reliability of the above Newton-Raphson solution procedure when applied to problems with substantial kinetics. This procedure consists of:

1. Ordering all kinetic reactions by the magnitude of the gross forward or reverse reaction rate
2. For each reaction seek the species equation in which it is most important
3. If its gross effect on the equation exceeds some fraction of the other terms in the equation, combine all equations affected by that reaction so as to introduce it into only one equation
4. Restructure that one equation so that the error is linear about the equilibrium state of the reaction
5. If a saddle point in the error equation is identified, alter the guesses to permit the procedure to search for a solution in a more likely solution domain
6 Utilize a damping scheme that constrains the corrections, ΔV_i, from oscillating and also from overcorrecting the variables, V_i.

This procedure has proven highly successful. It is difficult to sufficiently emphasize the importance of this reliability for coupled calculations within a grid structured problem.

4.1.3 Linearized Predictor - Corrector Procedure

For well-stirred or plug-flow reactor problems, which do not explicitly include diffusion, solution by the chemistry solver routine constitutes the final step in achieving an answer. For flame type problems, where axial diffusion is considered, the equations are still in error due to utilizing guessed values for the variables at downstream stations, n + 1. For these problems, a corrector step is added to the solution procedure to reduce to zero the error caused by using downstream guessed values for the variables in the equations.

At convergence, the chemistry solver iterative Newton-Raphson solution procedure has available a full set of derivatives of all of the variables with respect to the errors in the equations. Knowing explicitly the variation of the equation errors with respect to input variables, a matrix of derivatives of variables with respect to input variables (which include the guessed downstream quantities) can be constructed. Using the species expression, Equation (37), as an example, a linearized representation of the conservation equation about the current solution estimate, can be written in the following form.

$$\alpha_{i,c} = \alpha_{i,p} + \left(\frac{\partial \alpha_i}{\partial \alpha_j^\circ}\right)\left(\alpha_{j,c}^\circ - \alpha_{j,p}^\circ\right) \qquad (44)$$

where subscripts p and c refer to the predictor and corrector values respectively and the repeated j index implies summation. The superscript 0 defines a composite species concentration term which includes the guessed downstream species concentration plus the known upstream initial species concentration and various multiplying factors.* Equations 44 and a similar equation for h, $\tilde{h}$ and T are constructed for the entire grid. In matrix form, the resulting set of simultaneous equations covers a large sparse matrix in a block tridiagonal form. These equations are solved for the predictor values α_i^p, h^p, $\tilde{h}^p$ and T^p at all of the grid locations. If equations 37 and 38 are truly linear about the current solution estimate, the predictor values would satisfy all the equations and the final answer would be achieved. However, the equations are not linear and several iterations of the corrector step are required before a solution is found. Also, due to nonlinearties, it has been found that during the initial iterations, when the solution estimates are far from the answer, corrections to the variables must be limited to prevent overcorrections. The PROF procedure, which limits the variable corrections at each iteration, has proven to be adequate for all problems calculated.

Although flame solutions have been achieved by simply repeating the predictor step, the addition of the corrector step has been found to reduce the required number of iterations by factors of 2 to 10. Since Step 5 takes only 10 to 15 percent of the total computation time, it is a very effective method for reducing total computer run time. In addition to increasing computational speed, the corrector step allows the prediction of flame speed through the application of constraints on the grid variables. The flame speed, or mass flowrate, $\dot{m}$, is obtained by assigning a species concentration or temperature which is between the inlet and final equilibrium value, to

*Specifically it equals all $\alpha_{i_{n+1}}$ and $\alpha_{i_{n-1}}$ terms in Equation 37 divided by the coefficient on the α_{i_n} term.

a grid point removed from the inlet. The species constraint value may be assigned to any stable species which monotonically increases or decreases through the flame. The corrector step then updates the mass flowrate at each iteration until the assigned variable constraint is achieved at the specified grid point.

Summarizing the complete flame solution procedure, the set of algebraic equations found from the finite difference form of the species and energy equation are solved by the following steps:

1. Guessed initial values are selected for α_i, T, $\tilde{h}$ and h at grid points downstream of the first station. These are available as output from a prior run or are generated internally from a linear interpolation between initial and guessed final values.
2. Applying known upstream conditions and the initial guessed values, current grid point values for α_i, T and h, are found through matrix solution of the equation set in the chemistry solver routine.
3. When the downstream boundary is reached the no diffusion boundary condition is applied.
4. Utilizing the derivatives of α and T obtained from chemistry solutions at all grid points, the rate of change of all α_i's, $\tilde{h}$'s, h's and T's with respect to initially guessed a_i's, $\tilde{h}$'s and T's at each grid point are constructed.
5. The block tridiagonal matrix developed from Equation 44 and step 4 is solved simultaneously for all $\alpha_i{}^c$, $\tilde{h}^c$, h^c, T^c in terms of $\dot{m}^c$.

6. A constraint condition is then introduced to determine $\dot{m}_c$ and all other corrected variables. Using the corrected α_i's, $\tilde{h}$'s, h's and T's, as new guesses steps 2 through 6 are repeated until a converged solution is found.

4.2 Plug-Flow Reactor Solution Procedure

The plug-flow reactor algebraic equations are derived from the differential equations, Equations 28 and 29, utilizing the same linear finite differencing as was applied in the flame case (see Section 4.1.1). However, the distance, s, remains untransformed in the plug-flow reactor case. The finite difference plug-flow reactor governing equations are:

Species

$$Y_{i_n} - Y_{i_{n-1}} = \left[\frac{AW_i}{\dot{m}}\right]\left(\frac{S_{n+1} - S_{n-1}}{2}\right) - \frac{C_w}{\dot{m}} J_{w_i}\left(\frac{S_{n+1} - S_{n-1}}{2}\right) \tag{45}$$

Energy

$$h_n - h_{n-1} = -\left(\frac{S_{n+1} - S_{n-1}}{2\dot{m}}\right)\left(AQ_r + C_w q_w\right)_n \tag{46}$$

As indicated previously, these equations do not require any guesses for downstream species concentrations or enthalpy. Solution of this simple initial value problem is then found once the chemistry solver step, described in Section 4.1.2, is completed. Calculations over substantial lengths are carried out by repeating the above described step for either fixed or variable distance increments.

The time-evolution chemical kinetic problem is solved in a manner similar to the plug-flow reactor problem. However, in the time-evolution problem, the last term in Equation (45) is dropped and the parameter $\frac{A}{\dot{m}} \frac{S_{n+1} - S_{n-1}}{2}$, is replaced by a time increment divided by density, or $\frac{t_{n+1} - t_{n-1}}{\rho}$. In the time-evolution problem ρ is carried implicitly in the calculations.

4.3 Well-Stirred Reactor Solution Procedure

The well-stirred reactor solution procedure is equivalent to a single distance step of the plug-flow reactor procedure with $V/\dot{m}$ replacing the parameter $Ads/\dot{m}$ in equations (45) and (46). Typically the "time step" parameter $V/\dot{m}$ for the well-stirred reactor problem can be quite large relative to that typically employed for plug-flow reactor problems. This presents no special difficulty for the chemistry solution procedure. Sufficient convergence and rescue procedures have been incorporated into this routine to minimize nonconvergences due to starting with poor first guesses for the variables.

SECTION 5

CODE INPUT INSTRUCTIONS

This section fully describes the punched card input needed to activate the PROF code flame, well-stirred, plug-flow and time-evolution reactor options. A number of comments are included in this section to help guide the user in setting up input card decks. Comments specific to individual sample problems are given in Section 7.

5.1 Card Input Deck

Card 1		(Format 20A4)
1 - 80		Title of Run
Card 2		(Format 16I3) Integral Parameters
1 - 3	IS	Number of species conservation equations
4 - 6	KR6	Flag on type of solution to be obtained
	-1	Well-stirred reactor with assigned temperature of entering reactants
	0	Plug-flow reactor problem with distance as scale and assigned temperature of initial reactants
	1	Chemically reacting mixture with assigned temperature and pressure as a function of time
	2	Premixed flame problem with mean Lewis number of unity i.e. h = constant through flame for no radiation or specified heat loss (see ITC parameter description for heat loss option)
	3	Premixed flame problem, including nonunity Lewis number effects
7 - 9	N	Number of species (currently set N = IS)
10 - 12	NL	Number of axial grid points

13 - 15 NIT Number of grid solution corrector step iterations

16 - 18 INA Control on solution cycle

- 0 No effect
- 1 Punch α_i, etc. for subsequent input (see card set 9)
- 2 Read α_i, etc. (card set 9)
- 3 Punch and read α_i, etc.
- 4 Recycle calculation - stacked runs
- 5 Recycle and punch α_i, etc.
- 6 Recycle and read α_i, etc.
- 7 Recycle, read and punch α_i, etc.

19 - 21 IALF For first input deck IALF must be 1 or 2; but if IALF = 2, INA must = 2, 3, 6 or 7.

- 0 Do not read card set 7
- 1 Read card set 7 and set up interpolated α_i first guesses
- 2 Read card set 7 but do not set up subsequent first guesses

22 - 24 IAP

- 0 Do not read nonintegral parameters
- >0 Read nonintegral parameters (card set 3)

25 - 27 ITC

- 0 Do not read in thermochemical data
- >0 Read in linear fitted thermochemical data
- <0 Read in curve fitted thermochemical data

If ITC is nonzero, thermochemical data is read from a mass storage file designated as unit 12 for linear fit data and unit 11 curve fit data. The formats for this data are given in Section 5.2. Besides indicating what

		kind of thermochemical data is to be read, this parameter also identifies what kind of heat loss model is to be applied in the calculations.
	±1	No heat loss downstream of flameholder
	±2	Volumetric heat loss input as function of distance (card set 6)
	±3	Radiative volumetric heat loss
	±4	Convective heat loss to bounding walls (card set 6)
28 - 30	IFV	
	0	Do not apply constraint condition
	1	Flame calculation with constraint
31 - 33	IKN	
	0	Do not read in kinetic data. If this is the first of a stacked set of decks, no kinetics will be considered, otherwise previously read data will be used.
	>0	Read in kinetic data (card set 8)
34 - 36	IKAP	Variable to which constraint is applied. Used only in flame calculations i.e. IFV $\neq$ 0. 0 assigns a constraint on temperature; 1 to IS assigns a constraint on the corresponding species concentration (See card set 7 for order of species).
37 - 39	KAP	Grid point at which constraint is applied
40 - 42	KR7	Output control
	0	Final summary table and flame speed
	1	Detailed kinetics, molar fluxes of species, plus all of the above.
	2	Flame subroutine summary information, predictor/corrector matrix procedure information, and all of the above.
	3	All the above plus kinetic debug information
	>3	Complete debug printout

43 - 45 NFH Flameholder flag

0 No flameholder

1 Read and assign flameholder temperature at second grid point

2 Same as in NFH = 1 plus third body reactions are equilibrated at flameholder

46 - 48 MDOT Assigned mass flowrate flag

0 Flame speed calculation

1 Assign a fixed mass flowrate flame problem with a constraint condition

Card Set 3 Nonintegral Parameters

Card 1 (Format 8E10.5)

1 - 10 APR Composite "time scale" parameter

Well-stirred reactor (KR6 = -1):

$$APR = \left(\frac{V_o}{\dot{m}}\right)$$ Volume of reactor divided by the mass rate through the reactor ($cm^3 sec/gm$)

Plug-flow reactor (KR6 = 0):

$$APR = \frac{A_o}{\dot{m}}$$ Inverse of mass velocity ($cm^2 sec/gm$)

Time-evolution problem (KR6 = 1):

$$APR = \Delta t_o$$ Reference time step (sec)

Flame option (KR6 = 2 or 3):

For APR > 0 and MDOT = 0

$$APR = \frac{\delta A_o}{\dot{m}}$$

(See Section 4.1.1 for definitions of these terms. Section 7 gives instruction on how to construct this parameter).

For APR < 0 and MDOT = 0

The APR in storage from previous run is used in present run.

For APR > 0 and MDOT = 1

$$APR = \frac{\dot{m}}{A_o}$$

Mass flux ($gm/cm^2 sec$)

This is only for an assigned mass flux problem. Internally, APR reverts to MDOT = 0 definition after input sequence.

11 - 20 BP Composite diffusion parameter

Well-stirred reactor (KR6 = -1): BP = 0.

Plug-flow reactor (KR6 = 0): BP = 0.

Time-evolution problem (KR6 = 1): BP = 0.

Flame option (KR6 = 2 or 3): $BP = A_o\tilde{D}/\dot{m}\delta$ (See Section 4.1.1 for definition of these terms. Section 7 gives instructions on how to construct this parameter).

21 - 30 P Pressure (atm) (This value is replaced in assigned P and T time-evolution problem by PPB input. (See card set 5)).

31 - 40 T Initial temperature (K). (This value is replaced in assigned P and T time-evolution problem by TTB input. (See card set 5)).

41 - 50 TKAP	Value of constraint variable. Can be temperature, in K degrees, or any monotonically increasing or decreasing major species concentration, in mole/gm units. This constraint condition is only used with flame calculations. The code will adjust the flame speed or grid spacing until the constraint variable is achieved at grid point KAP.
51 - 60 TFLAME	Assigned flameholder and gas temperature in °K at the second grid point. For well-stirred reactor calculations TFLAME is used as the first guess for reactor temperature.
Card Set 4	Spatial or Temporal Grid Parameters for points N = 1, NL
Card(s) 1	(Format 8E10.4)
1 - 10, 11 - 20,..AP(N)	Time or area parameter Well-stirred option (KR6 = -1) Ratio of reactor volumes, V/V_o. AP(1) is not used, start with AP (2) Time-evolution problem (KR6 = 1) Ratio of grid point time step to the reference time step, $\Delta t/\Delta t_o$, AP(1) is not used, start with AP(2). Plug-flow option (KR6 = 0) and flame option (KR6 = 2 or 3) Area ratio A/A_o at each grid point.
Card(s) 2	(Format 8E10.4)
1 - 10, 11 - 20,..DS(N)	Space step parameter Plug-flow option (KR6 = 0) Relative grid spacing along flow axis in cm.

Time-evolution (KR6 = 1) and well-stirred option (KR6 = -1)
Set equal to 1.

Flame option (KR6 = 2 or 3)
Relative normalized grid spacing along flow axis. (See Section 4.1.1 for definition of DS(N)).

Card Set 5 — Assigned Temperatures and Pressures for Fixed Mass Time-Evolution Problems (KR6 = 1)

Card(s) 1 — (Format 8E10.5)

1 - 10, 11 - 20,TTB(N)	Temperature in °K at station N for NL stations

Card(s) 2 — (Format 8E10.5)

1 - 10, 11 - 20,PPB(N)	Pressure in atm. at station N for NL stations

Card Set 6 — Heat Loss Options

Option I - Volumetric heat loss (ITC ±2)

Card(s) 1 — (Format 14, 6X, E10.5)

1 - 4 INS	Number of heat loss entries to be specified as a function of axial distance.
11 - 20 QLS	Volumetric heat loss (cal/cm^3 sec) If INS is greater than one then local Q values referenced to the QLS above will be input as a function of axial distance.

Card(s) 2 — (Format 8E10.5)

1 - 10, 11 - 20,SSS(N)	Only for INS > 1. Distances in cm which Q local to QLS ratios are specified; 1 to INS ratios are required.

Card(s) 3 (Format 8E10.5)

1 - 10, 11 - 20,	Q/Q(N)	Local Q to QLS ratios specified as a function of axial distance. 1 to INS entries required.

Option II - Convective transfer coefficient input (ITC ±4)

Card 1 (Format I4, 6X, E10.5)

1 - 4	INS	Number of heat transfer factor entries
11 - 20	Cj	Transfer coefficient constant for J factor (see Section 3.1.3).

Card(s) 2 (Format 8E10.5)

1 - 10, 11 - 20,	SSN(N)	Distances in cm at which transfer coefficient values are specified.

Card(s) 3 (Format 8E10.5)

1 - 10, 11 - 20,	Q	Local values of $Q = 1/D_h L^m$ at SSS, consisting of the hydraulic diameter, D_h, and the Reynolds number reference length, L used in Equation 13. For well-stirred reactors D_h is four times volume/surface area and for plug-flow reactors and flames D_h is four times sectional area/perimeter.

In addition to the general formulation of Equation 13, two limiting cases of specific interest are:

Assigned J factor as a function of distance: let C_J° = reference J factor, m = 0 and $Q = J/(D_h C_J^\circ)$

Assigned Nusselt Number: let C_J° = reference Nusselt number, m = n = 1, and $Q = Nu/D_h^2 \cdot Nu^\circ$).

Card(s) 4 (Format I4, 6X, 3E10.5)

1 - 4	IH	Wall reactivity parameter
	1	Noncatalytic wall
	2	Reactive wall - composition to be specified

3	Same as 2 but adiabatic wall
11 - 20 TW	Wall temperature (°K)
21 - 30 EXM	Exponent m of Equation 13
31 - 40 EXN	Exponent n of Equation 13
Card(s) 5	(Format 8E10.5)
1 - 10, 11 - 20, PW(N)	Wall species relative mole concentrations (should yield same elemental composition as the bulk gas phase). Species order is the same as on card set 7. This input is not needed when IH=1.
Card Set 7	Initial species concentrations, downstream species concentration guesses, species diffusion factor's and equivalent species names.
Card(s) 1 to IS	(Format 2A4, I2, 2E10.3, F10.4)
1 - 8 NAMA	Species name utilized in kinetic reaction input. (These names must also be compatible with or equivalent to (see card(s) IS±2 in this card set) the names on the thermochemical input data tape). See Section 5.2 for a description of thermochemical data.
11 - 20 ALPHF	Initial species concentration in relative mole concentrations.
21 - 30 ALPHE	Estimate of terminal species concentrations in relative mole concentrations. Input should approximate maximum value achieved in flame for initial trace quantities. This input is overridden if first guesses are input from prior run. (See card set 9 for a description of this input).
31 - 40 BPA	Bifurcation diffusion factors, $1/F_i$, for each species. See Section 3.1.1 for the definition of these factors. These are not needed for nonflame and nonwall loss calculations. For these cases a value of one may be input.

Card IS + 1	(Format 2A4)
1 - 3	Input of END signifies the end of the species input set
9 - 10 KNY	Number of equivalent species name cards to follow
Card(s) IS + 2	(Format 2A4, 2X)
(Col) 1 - 8, NAMA 21 - 28, 41 - 48, or 61 - 68	Species name used in thermochemical input data file
(Col) 11 - 18, NAMC 31 - 38, 51 - 58, 71 - 78	Species name equivalenced to NAMA. Can be name on species or reaction input which does not match thermochemical input data file name.
	Four equivalenced sets of names may appear on each card with a maximum of four cards being read. No species name can occur in more than one equivalence set.
Card Set 8	Kinetic Data

If IKN > 0 this data must be present. For IKN = 0, the reaction data stored during previous input is used in calculations. Reactions and their associated rates are given in the form:

$$A + B + M \rightarrow C + D$$

where M denotes a general third body.

The forward rate coefficient is given by:

$$k_f = AT^b e^{-\frac{Ea}{RT}} \quad \text{(mole-cm-sec units)}$$

The reverse rate is obtained through use of the equilibrium constant and the forward rate. (The species names must be compatible with or equivalent to those on the thermochemical input data tape and initial species concentration input data).

Card 1		(Format 13)
1 - 3	MT	The number of reactions and rate coefficients to be input
Card(s) 2		(Format 5 (A4, 1X), 5X, 3E10. 4, 2(A4, F6.1))
1 - 4, 6 - 9	NAMA	Name of reactants (e.g. H, O, H2, O2 etc.)
11 - 14	M	General third body (Enter M) or specific third body (e.g. H, O, H2, O2, etc.)
16 - 19, 21 - 24	NAMA	Name of products (e.g. H, O, H2, O2, etc.)
26 - 30		$\mathrm{Log}_{10} A_0$, where A is pre-exponential factor in mole-cm sec units
31 - 40	A/A_0	Pre-exponential factor Note $\log_{10}$ of this value added to entry in col. 26-30. For $A_0 = 1.0$ no entry is required in columns 26-30.
41 - 50	b	Temperature exponent
51 - 60	Ea	Activation energy in Kcal/gm mole units
61 - 64, 71 - 74	NT	Individual third body name (e.g. H,O etc.)
65 - 70, 75 - 80	TB	Individual third body efficiencies (i.e. rate with specific third body is TB times the rate associated with the general third body. TB should be one less than the specific third body rate since M already includes the individual third body).
Card Set 9		Initial guesses for flame species concentrations and velocity (INA = 2, 3, 6, 7). If present, these guesses replace those obtained from card set 7.
Card 1		(Format 20A4)
1 - 80		Title run in which the following input data was generated

Card 2 (Format 2I3, 3E10.5)

1 - 3	NS	Number of grid points in first guess input
4 - 6	NIS	Number of species in first guess input. The order of species must be the same as in card set 7.
7 - 16	APRR	If nonzero and MDOT = 0, this entry overrides the APR value input in card set 3 and becomes the first guess for the flame speed parameter (see Section 4.1.1 for the definition of this term.)
17 - 26	BPR	If nonzero, this entry becomes the value for BP and overrides entry in card set 3. (See Section 4.1.1 for the definition of this term).

Card(s) 4 (Format 10E8.4)

1 - 8, 9 - 16, 17 - 24	DSS(N)	Normalized grid spacing parameter for species input (NS values input). Same definition as given in card set 4.

Card(s) 6 (Format 10E8.4)

1 - 8, 9 - 16	HI(N)	Grid enthalpies in (cal/gm) units. NS-1 values must be input covering stations 2 through NS.

Card(s) 7 (Format 10E8.4)

1 - 8, 9 - 16	ALA(I,N)	Grid species concentrations in (mole/gm) units. NS-1 values must be input covering stations 2 through NS. NIS number of species input.

5.2 Thermochemical Input Data Format

For program operation, thermochemical data (i.e. specific heat, enthalpy and entropy) for all species included in card set 7 (given in Section 5.1) must be present on mass storage devices designated by unit 12 for tabular format and unit 11 for curve fit format. The order of this data on the storage device is not important. However, it is important that the species names input on card set 7 match identically with or are equivalenced to the species names on the thermochemical data files and the kinetic reaction input data, card set 8. The thermochemical data files can be full libraries of data, from which only a limited number of species will be selected for each problem of interest. Revisions or additions to this library can be made utilizing the TCUP program which is described in Section 5.3.

As indicated in Section 5.1, either tabular or curve fit thermochemical data can be utilized by the code. If ITC is greater than zero on card 2 (see Section 5.1) then tabular data is required by the code. For each species of interest the following 31 data cards must be present on unit 12.

Card 1	(Format 10X, 2A4, 2X, 2F10.1)
11 - 18 NAMA	Species name utilized in initial concentration and reaction input
21 - 30 MW	Molecular weight of species
31 - 40 HRF	Heat of formation of species at 298°K (Cal/mole)
Cards 2 - 11	(Format 5 (1X, E12.5))
2 - 10, 12 - 20, ...CP	Specific heat every 100°K from 100°K to 5000°K (cal/mole°K)
Cards 12 - 21	(Format 5 (1X, E12.5))
2 - 10, 12 - 20, ...$H-H_{298°K}$	Enthalpy difference referenced to 298°K every 100°K from 100°K to 5000°K (Kcal/mole)

Cards 22 - 31 (Format 5 (1X, E12.5))

2 - 10, 12 - 20,.	$F = (G-H_{298^\circ})/T$. Function related to free energy every 100°K from 100°K to 5000°K (cal/mole°K).

If ITC is less than zero on card 2 (see Section 5.1) then curve fit data is required by the code. For each species of interest the following 3 data cards must be present on unit 11.

Curve fits of data are in the form $Cp = F_3 + F_4T + F_5/T^2$ and cover a lower and upper temperature range.

Card 1 (Format 10X, 2A4, 2X, 2F10.0)

11 - 18	NAMA	Species name utilized in initial concentration and reaction input
21 - 30	MW	Molecular weight of species

Card 2 (Format 6E9.6, 6X, F6.0, 6X, A4)
Low temperature curve fit.

1 - 9	F_1	Heat of formation at 298°K (cal/mole)
10 - 18	F_2	Change in enthalpy from 298°K to 3000°K (cal/mole)
19 - 27	F_3	Coefficient in above Cp expression
28 - 36	F_4	Coefficient in above Cp expression
36 - 45	F_5	Coefficient in above Cp expression
46 - 54	F_6	Entropy constant at 3000°K (cal/mole)
61 - 66	TU	Upper temperature limit of low temperature range curve fit (°K)
73 - 76	NAMA	Name of species used in reaction set

Card 3 (Same format as above)

High temperature range curve fit. Same data as above for temperatures beginning at the maximum of the above data.

5.3 PROF Thermochemical Data Update Program (TCUP)

The TCUP program, described in this section, updates and expands the PROF code curve fit or tabular thermochemical data files. Another option lists the complete thermochemical data file.

The program accepts only a list or update directive and checks to see if the CURVE FIT or TABULAR data master file is assigned. The program terminates if the directive is not correct or the data file is not found.

5.3.1 List Option

The program gives a complete listing of the contents of the master file and indicates the number of species present. The master file should be assigned to unit 11. Only one card is required for a list.

Card 1	(Format A2, 8X, 2A4)
Col. 1 - 10	(Starting in Col. 1) LIST or LI
Col. 11 - 18	(Starting in Col. 11) CURVE FIT or CU, TABULAR or TA for type of data to be listed

5.3.2 Update Option

The program adds, changes, and deletes whole records. (i.e. 3 cards of curve-fit data and 31 cards of tabular data for each species).

Three files must be assigned.

1) The old master file on unit 11
2) The new master file on unit 12
3) A scratch file on unit 10

An update directive is established by the following card.

Card 1	(Format A2, 8X, 2A4)
Col. 1 - 2	(Starting in Col. 1) UPDATE or UP
Col. 11 - 18	(Starting in Col. 11) CURVE FIT or CU, TABULAR or TA for type of data to be updated

Update Control Cards

One card is required for each set of species data being updated. Only one update to a species can be made in each run. If there is more than one update to a species, only the first update will be carried out.

Additions to the file are activated by the following control card:

Card 2 (Format A2, 8X, 2A4)

Col. 1 - 2 *ADD or *A

Program adds following species data to the current data file. The program checks to see if the species already exists and if so, no additions are made. The new species data is added onto the end of the master file.

Card Set 3 Thermochemical Input Data

Species identification and data card

Card 3 (Format 10X, 2A4, 2X, 2F10.0)

Col. 11 - 14 NAMA Species name utilized in reaction input

Col. 21 - 30 MW Molecular weight of species

Col. 31 - 40 HRF Heat of formation of species at 298°K (cal/mole)

For tabular data, the thermochemical information must be entered in the following form:

Cards (4 - 13) (Format 5 (1X, E12.5))

Col. 2 - 10, 12 - 20 CP Specific heat every 100°K from 100°K to 5000°K (cal/mole°K)

Cards (14 - 23) (Format 5 (1X, E12.5))

Col. 2 - 10, 12 - 20, $H-H_{298°K}$ every 100°K from 100°K to 5000°K (Kcal/mole)

Cards (24 - 33) (Format 5 (1X, E12.5))

Col. 2 - 10, 12 - 20, $F = (G-H_{298°})/T$. Function related to free energy every 100°K from 100°K to 5000°K (cal/mole°K)

For curve fit data, the thermochemical information must be entered in the following form, where $CP = F_3 + F_4T + F_5/T^2$:

Card 4		(Format 6E9.6, 6X, F6.0, 6X, A4)
		Low temperature range curve fit
Col. 1 - 9		F_1 Heat of formation at 298°K (cal/mole)
Col. 10 - 18		F_2 change in enthalpy from 298°K to 3000°K (cal/mole)
Col. 19 - 27		F_3 Coefficient in above Cp expression
Col. 28 - 36		F_4 Coefficient in above Cp expression
Col. 37 - 45		F_5 Coefficient in above Cp expression
Col. 46 - 54		F_6 Entropy constant at 3000°K (cal/mole°K)
Col. 61 - 66		TU upper temperature limit of low temperature range curve fit (°K)
Col. 73 - 76	NAMA	Name of species used in reaction set
Card 5		(Format 6E9.6, 6X, F6.0, 6X, A4)
		High temperature range curve fit. Same data as above for temperatures beginning at the maximum of the above data.

The following instructions must be present to replace current species data on the file with new data:

Card 2	(Format A2, 8X, 2A4)
Col. 1 - 2	(Starting in Column 1) *CHANGE or *C
Card Set 3	The change instruction must be followed by curve fit or tabular data in the same format as given under the add option described above.

The following instruction must be present to delete current species data on the file:

Card 2	(Format A2, 8X, 2A4)
Col. 1 - 2	(Starting in Column 1) *DELETE or *D
Col. 11 - 14	(Starting in Column 11) NAMA species - name which is to be deleted. This name must match that used on the file. If no name is given then the delete command is not carried out.
Last card	(Format A2, 8X, 2A4)
Col. 1 - 2	(Starting in Column 1) *END or *E. This card ends the update process.

SECTION 6

OUTPUT

The PROF code output gives complete summary information for flame, well-stirred and plug-flow reactor and time-evolution chemical kinetic problems. If called for, it can also provide information on intermediate iterations and chemistry routine solutions. For each iteration during a flame solution the code always prints out a line of output which gives the flame speed parameter, its error, the maximum error in concentration and the constraint (i.e. damping) applied to the corrector step correction vector. In addition, all of the input data is output along with the title of the run.

Debug output can be activated by assigning KR7 equal to or greater than three. The meaning of this output is discussed in Section 8. The following subsections describe a typical nondebug output.

6.1 Integral and Nonintegral Input Parameters

The first (or more) page of output lists the run title, integral parameters, nonintegral grid parameters, assigned pressures and temperatures and wall heat loss data. This output is listed in the same order in which it is read in on card input, and is simply a printing of the input information with notations to clearly indicate what has been read. Examples of this output for several sample problems are given in Section 7.

6.2 Species Names and Concentrations

The next page of output lists the species names, initial mole fractions, guesses of final mole fractions and the diffusion factors for the individual species. This output is clearly labeled and is simply a listing of output.

6.3 Thermochemical Data

The next page(s) of output is a listing of the thermochemical curve fit or tabular data obtained from the thermochemical data file for each species. If curve fit data is specified, three lines of output giving the species name and molecular weight, curve fit and other constants appears for each species. For tabular data, 31 lines of output giving specific heat, enthalpy and free energy for each species appears. This information, which is clearly labeled, is completely described in Section 5.2.

6.4 Kinetic Reaction Data

On this page of output a completely labeled listing of kinetic reaction input data is given along with the associated reaction rates.

6.5 First Guess Alphas

If punched card output from a prior run is used as first guesses, the values read in will be output in this section. Information given includes, the normalized distance coordinate used in the prior run and the enthalpy and species concentration distributions obtained in the prior run. In addition to this listing of input data, the enthalpy and species concentrations scaled from the input to the problem being calculated are also output. These values are assigned to the grid points as first guesses.

6.6 Chemistry Solutions at Grid Points

If KR7 is 2 or greater chemistry solution output is printed at each grid point. Information given in this output includes, the number of interations required to achieve a converged chemistry, the grid point index, pressure mixture molecular weight product, temperature in degrees K, and partial pressures of the IS species in atmospheres. Output corresponding to the NL grid points are given in this section of output.

6.7 Condensed Output for Each Iteration

For flame problems where KR7 is 2 or greater, values of alpha (species concentrations, enthalpy and for problems where KR6 = 3, temperature and enthalpy tilda) as predicted in the chemistry routine are output followed by values of alpha determined in the corrector step. Descriptions of the procedures used to obtain these values are given in Sections 4.1.2 and 4.1.3. The degree of convergence of the flame solution is indicated by the relative difference between the predictor and corrector alphas at each grid point. When the predicted alphas equal the corrected alphas the solution is converged.

Following the predictor and corrector alphas is a single line of output giving the flame speed parameter, APR, the predicted correction in this parameter, DAPR, the maximum alpha error found for the entire grid, and the constraint on the corrector step correction vector. This constraint multiplies the correction vector and prevents over corrections from being made to the variables.

6.8 Mole flux at grid points

On the final iteration of a flame solution problem, the code prints out the reaction creation, diffusion flux out and convective flux out for each species at all grid points. These appear underneath one another and are in units of mole/cm^2/sec. The grid point number at each station is printed out along with the nodal width in centimeters for that station. The creation and sum of the flux terms at each end point will only balance if the solution is converged.

6.9 Grid Information Summary Table

This section of output always appears and provides final information for flame, well-stirred reactor, plug-flow reactor and time-evolution chemical kinetic problems. The first line of output gives the number of iterations and how many grid points are being calculated. For flame calculations, the flame speed parameter, APR, is printed out along with the associated flame speed in cm/sec. It should be noted that for a flame problem which is not yet converged (i.e. DAPR is a considerable fraction of APR and maximum relative alpha error is greater than 0.001 in final output described in Section 6.7), these parameters, plus all subsequent output, only represent intermediate values and have no physical significance. The grid coordinates output for NL grid points are the distances, in cm, between nodes defined by s on page 4-2. These are the coordinates which can be used in plotting gas properties. For time-evolution and well-stirred reactor problems this output does not apply. The nondimensional grid coordinates are the nodal widths used to develop the grid coordinates and time. These are input parameters. Like the grid coordinate output, the time output is the time in seconds between nodes. For well-stirred reactor problems this output gives the residence time in reactor for each reactor calculation. Following the coordinate information is gas enthalpy (cal/gm), temperature (K), density (gm/cm^3), system molecular weight and species concentration for the NL grid points. This information is strung out eight grid points to a line until NL grid points are covered.

6.10 Kinetic Reaction Summary Information

If KR7 is greater than zero, detailed information on the kinetic reaction rates are output in this section. The first block of output gives the forward kinetic production rate of each reaction in mole/cm^3/sec at each grid point. This information is strung out eight grid points to a line until NL grid points are covered. The second block of output gives the ratio of the forward to backward rate of each reaction. A value near one indicates that the reaction is approaching equilibrium. This output is also strung out eight grid points to a line until NL grid points are covered. The third block of output lists, for each grid point, the reactions and rates, in mole/cm^3/sec units which contribute to the formation of the individual species. This output can be used to assess the importance of various reactions to the chemical evolution of the problem. If a reaction does not contribute significantly to any species formation or depletion over the entire grid, then this reaction can be extracted from the calculation without significantly affecting the results.

SECTION 7

SAMPLE CASES

A total of five sample cases are discussed in this section. These cases illustrate how the flame, well-stirred reactor, plug-flow reactor and time-evolution chemical kinetic problem input decks are set up and what type of output is to be expected when these problems are run. Listings of the input cards along with selected sections of output are given for each case.

7.1 Sample Case 1 - Free Methane/Air Flame

The free flame case, described presently, and the attached flame problem, which will be discussed subsequently (Section 7.2), are the primary options of the PROF code. As mentioned previously for the free flame case, the elementary chemical kinetic and transport data input into the code along with the initial conditions define flame speed. Within the bounds of flammability, the code will always determine a flame speed consistent with the input data. In the case of the attached flame problem, mass flowrate of reactants is assigned. In some instances, the assigned flowrate is inconsistent with the chemical kinetic and transport data input into the code. Under these conditions no stationary nontrivial flame solution will exist and the code will fail. To avoid this problem, a free flame calculation should be performed prior to an attached flame calculation. The mass flowrate corresponding to the predicted flame speed can then be compared to the potential assigned flowrates. If the former flowrate is less than an assigned mass flow, no stationary solution exists and the flame will be "blown off." For these cases, either the assigned flowrate or the kinetic and transport data must be adjusted before a nontrivial attached flame

SAMPLE PROBLEM 7.1

```
  1.    CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.952
  2.    16  3 16 25  8  3  1  1 -3  1  1  1 12  2
  3.   .036671   .25       1.0       298.      .002
  4.   1.        1.        1.        1.        1.        1.        1.        1.
  5.   1.        1.        1.        1.        1.        1.        1.        1.
  6.   1.        1.        1.        1.        1.        1.        1.        1.
  7.   1.        1.        1.        1.        1.        1.        1.        1.
  8.    .5        .3        .2        .1        .05       .05       .05       .05
  9.    .05       .05       .05       .05       .05       .05       .1        .1
 10.    .2        .5        .5       1.0       1.0       2.0       2.0       4.0
 11.    4.0
 12.   CH4       .091                1.-31.0523
 13.   O2        .191                1.-31.0468
 14.   CO2             1.-9.1              .8
 15.   H2O             1.-9.06         1.2980
 16.   H2              1.-9      1.-33.5333
 17.   CO              1.-9      1.-3 .9830
 18.   CH3             1.-9      1.-31.3257
 19.   CH2O            1.-9      1.-31.2980
 20.   CHO             1.-9      1.-3 .9604
 21.   HO2             1.-9      1.-3 .9016
 22.   H               1.-9      1.-35.1557
 23.   O               1.-9      1.-31.4158
 24.   HO              1.-9      1.-31.3475
 25.   N2        .718      .718       .9732
 26.   CH              1.-9      1.-31.43
 27.   CH2             1.-9      1.-31.37
 28.   END
 29.    37
 30.   CH4       M   CH3  H           1.50+18     0.       100.0
 31.   CH4  HO       CH3  H2O         1.00+13    0.0       6.000
 32.   CH4  H        CH3  H2          2.00+14    0.0      11.900
 33.   CH4  O        CH3  HO          2.00+13    0.0       6.900
 34.   CH3  O        CH2O H           3.50+13    0.0       3.300
 35.   CH3  O2       CH2O HO          1.00+12    0.0      15.000
 36.   CH2O      M   CO   H2          2.00+16    0.0      35.000
 37.   CH2O HO       CHO  H2O         2.50+13    0.0       1.000
 38.   CH2O O        CHO  HO          3.00+13    0.0       0.
 39.   CH2O H        CHO  H2          1.70+13    0.0       3.000
 40.   CHO  O2       CO   HO2         3.00+13    0.0       0.
 41.   CHO  HO       CO   H2O         1.00+14    0.0       0.
 42.   CHO  O        CO   HO          5.40+11    0.5       0.
 43.   CHO       M   CO   H           2.00+12    0.5      28.800
 44.   CO   HO       CO2  H           5.50+11    0.0       1.080
 45.   CO   O    M   CO2              3.60+18   -1.0       2.500
 46.   HO2  O        O2   HO          2.50+13    0.0       0.
 47.   HO2  HO       O2   H2O         2.50+13    0.0       0.
 48.   HO2  H        HO   HO          2.50+14    0.0       2.000
 49.   HO2  H        O2   H2          2.50+13    0.0        .000
 50.   H    O2   M   HO2              2.00+15    0.0        .870   H2O  20.
 51.   H    O2       HO   O           2.20+14    0.0      16.800
 52.   O    H2       HO   H           1.70+13    0.0       9.460
 53.   HO   H2       H2O  H           2.20+13    0.0       5.200
 54.   HO   HO       H2O  O           6.00+12    0.0        .780
 55.    H     HO    M     H2O               7.00+19   -1.0      0.
 56.    O     H     M     HO                4.00+18   -1.0      0.
 57.    H     H     M     H2                2.00+19   -1.0      0.
 58.    O     O     M     O2                4.00+18   -1.0      0.
 59.    CH3   HO          CH2   H2O         6.00+09          .7       2.0
 60.    CH2   HO          CH    H2O         5.00+11          .5       6.0
 61.    CH2   O2          CH2O  O           5.00+11          .5       7.
 62.    CH    O2          CHO   O           5.00+11          .5       6.0
 63.    CH2   O           CHO   H           5.00+11      .5       4.0
 64.    CH    HO          CHO   H           5.00+11      .5      10.0
 65.    CH    O           CO    H           5.00+11      .5       4.0
 66.    CH2   H           CH    H2          3.00+11      .7      26.0
 67.     CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.952
 68.     25 16 .40331-01 .25000+00
 69.    .5       .3       .2       .1       .05      .05      .05      .05      .05      .05
 70.    .5000-01.5000-01.5000-01.5000-01.1000+00.1000+00.2000+00.5000+00.5000+00.1000+01
 71.    .1000+01.2000+01.2000+01.4000+01.4000+01
 72.    -.604+02-.604+02-.594+02-.580+02-.569+02-.555+02-.539+02-.519+02-.497+02-.472+02
 73.    -.446+02-.419+02-.396+02-.381+02-.400+02-.497+02-.639+02-.635+02-.609+02-.599+02
 74.    -.591+02-.589+02-.588+02-.587+02
 75.    .3211-02.3130-02.3018-02.2920-02.2850-02.2765-02.2663-02.2540-02.2391-02.2213-02
 76.    .2000-02.1749-02.1459-02.1139-02.5332-03.1403-03.8115-05.3037-06.1238-07.5227-09
 77.    .2185-10.8520-12.2843-13.7919-15
 78.    .6779-02.6655-02.6487-02.6341-02.6239-02.6116-02.5970-02.5797-02.5590-02.5345-02
 79.    .5053-02.4709-02.4305-02.3840-02.2837-02.1871-02.1065-02.7948-03.6733-03.5866-03
 80.    .5256-03.4812-03.4503-03.4309-03
 81.    .1153-04.2890-04.5796-04.8712-04.1090-03.1363-03.1705-03.2131-03.2661-03.3322-03
 82.    .4140-03.5151-03.6389-03.7894-03.1141-02.1560-02.2204-02.2575-02.2738-02.2856-02
 83.    .2941-02.3009-02.3056-02.3087-02
 84.    .2189-03.4226-03.6849-03.8977-03.1037-02.1197-02.1383-02.1597-02.1843-02.2126-02
 85.    .2449-02.2815-02.3225-02.3675-02.4585-02.5341-02.5840-02.6004-02.6131-02.6239-02
 86.    .6314-02.6365-02.6401-02.6422-02
 87.    .1495-03.2009-03.2473-03.2760-03.2920-03.3088-03.3267-03.3456-03.3656-03.3868-03
 88.    .4091-03.4324-03.4558-03.4780-03.5083-03.4855-03.3734-03.2982-03.2429-03.1850-03
 89.    .1457-03.1147-03.9449-04.8167-04
 90.    .2435-04.5410-04.9801-04.1376-03.1653-03.1984-03.2383-03.2861-03.3435-03.4122-03
 91.    .4944-03.5922-03.7075-03.8410-03.1123-02.1304-02.1030-02.6998-03.5438-03.4271-03
 92.    .3444-03.2772-03.2303-03.1999-03
 93.    .1134-04.2196-04.3609-04.4849-04.5762-04.6921-04.8393-04.1024-03.1251-03.1528-03
 94.    .1857-03.2229-03.2609-03.2919-03.2890-03.1606-03.1801-04.9666-06.4494-07.1811-08
 95.    .6829-10.2345-11.7027-13.1799-14
 96.    .1033-05.2046-05.3443-05.4609-05.5367-05.6217-05.7159-05.8200-05.9371-05.1072-04
 97.    .1230-04.1406-04.1572-04.1659-04.1329-04.6032-05.4928-06.1324-07.3431-09.9178-11
 98.    .1066-11.5619-12.3825-12.2874-12
 99.    .1468-11.9261-11.3293-10.6421-10.5894-10.2805-10.2149-10.1386-09.5622-09.1731-08
100.    .4844-08.1327-07.3565-07.8995-07.3312-06.4929-06.9734-07.5350-08.1360-08.7982-09
101.    .5414-09.3769-09.2856-09.2354-09
102.    .2175-06.7213-06.1661-05.2430-05.2801-05.3070-05.3202-05.3207-05.3136-05.3064-05
103.    .3065-05.3187-05.3411-05.3608-05.3064-05.1462-05.2783-06.1340-06.9411-07.6491-07
104.    .4599-07.3301-07.2529-07.2093-07
105.    .4782-11.3798-10.3956-09.2107-08.4409-08.7727-08.1206-07.1420-06.9069-06.2184-05
106.    .4276-05.7723-05.1349-04.2319-04.6039-04.1236-03.1885-03.1326-03.8513-04.5035-04
107.    .3229-04.2114-04.1509-04.1178-04
108.    .1880-09.6446-09.1717-08.3000-08.3328-08.3034-08.2407-08.1853-08.3531-07.1334-06
109.    .3738-06.9750-06.2434-05.5819-05.2402-04.6672-04.1154-03.8699-04.6052-04.3986-04
110.    .2797-04.2011-04.1549-04.1283-04
111.    .3575-09.1073-08.2809-08.5295-08.6660-08.7641-08.8406-08.1600-06.5838-06.1274-05
```

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112.    .2534-05,5049-05.1019-04,2033-04,6352-04,1412-03,2476-03,2558-03,2338-03,2019-03
113.    .1762-03.1536-03.1374-03.1265-03
114.    .2588-01,2587-01.2589-01.2591-01.2592-01.2593-01.2594-01.2595-01.2597-01.2598-01
115.    .2600-01,2601-01.2601-01.2600-01.2600-01.2597-01.2597-01.2595-01,2594-01,2594-01
116.    .2593-01,2593-01.2593-01.2593-01
117.    .6990-09,1839-08,3679-08,4807-08,4786-08,3820-08,2572-08,1332-08,7816-09,3660-09
118.    .1901-09,4019-09.1455-08,5250-08,3904-07,1415-06,9501-07,9348-08,5035-09,1864-10
119.    .6065-12,1746-13,4491-15,1024-16
120.    .1135-07,2250-07.3519-07,4098-07,4092-07,3798-07,3369-07,3147-07,3568-07,5183-07
121.    .8926-07,1676-06,3245-06,6137-06.1628-05,2150-05,5194-06,3478-07,1637-08,6072-10
122.    .2083-11,6469-13,1782-14,4282-16
```

```
                    PREMIXED ONE DIMENSIONAL FLAME CODE SOLUTION (PROF)

                  PROGRAM DOCUMENTED IN THE "PROF CODE USER'S MANUAL",
                    AEROTHERM/ACUREX CORP FINAL REPORT 78-277
                             PHONE 415/964-3200


   CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.952

                            * INTEGRAL PARAMETERS *

 COLUMN                                         COLUMN
    3  NO. SPECIES CONSERVATION EQS.  16            6  PROBLEM TYPE AND ENERGY EQ.      3

    9  NO. OF SPECIES                 16           12  NO. AXIAL GRID PTS.             25

   15  NO. GRID SOLUTION ITERATIONS    8           18  SOLUTION CYCLE CONTROL NO.       3

   21  READ INITIAL MOLE FRACTION      1           24  READ NONINTEGRAL PARAMETERS      1

   27  THERMO DATA & HEAT LOSS MODEL  -3           30  CONSTRAINT SWITCH                1

   33  READ KINETIC DATA               1           36  CONSTRAINT APPLIED TO VARIABLE   1

   39  CONSTRAINT APPLIED TO GRID PT. 12           42  OUTPUT CONTROL NO.               2

   45  FLAMEHOLDER TEMP ASSIGN SWITCH  0           48  INPUT MASS FLOWRATE SWITCH       0


                            * NONINTEGRAL PARAMETERS *

   APR=DEL/MDOT= .36671-01   BP=DBAR/(DEL*MDOT)= .25000+00    P=   1.000(ATM)   TI=   298.0(K)

        TKAP=    .00200   TFLAME=     .0(K)



                            * GRID PARAMETERS *

      A(N)**2 ,N=1, 25

       .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
            .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
                 .1000+01  .1000+01  .1000+01  .1000+01  .1000+01

       SIGMA(N),N=1, 25

       .5000+00  .3000+00  .2000+00  .1000+00  .5000-01  .5000-01  .5000-01  .5000-01  .5000-01  .5000-01
            .5000-01  .5000-01  .5000-01  .5000-01  .1000+00  .1000+00  .2000+00  .5000+00  .5000+00  .1000+01
                 .1000+01  .2000+01  .2000+01  .4000+01  .4000+01
```

```
* SPECIES INITIAL MOLE FRACTIONS.FIRST GUESSES.AND DIFFUSION FACTORS *

SPECIE          ALPF          ALPE        DIFFUSION FACTOR

CH4           .910-01       .100-02          1.0523
O2            .191+00       .100-02          1.0468
CO2           .100-08       .100+00           .8000
H2O           .100-08       .600-01          1.2980
H2            .100-08       .100-02          3.5333
CO            .100-08       .100-02           .9830
CH3           .100-08       .100-02          1.3257
CH2O          .100-08       .100-02          1.2980
CHO           .100-08       .100-02           .9604
HO2           .100-08       .100-02           .9016
H             .100-08       .100-02          5.1557
O             .100-08       .100-02          1.4158
HO            .100-08       .100-02          1.3475
N2            .718+00       .718+00           .9732
CH            .100-08       .100-02          1.4300
CH2           .100-08       .100-02          1.3700
```

```
                 * THERMOCHEMISTRY DATA *

          CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)  H(CAL/MOL)     RB          RC          RD      S(CAL/MOL/K)     TU(K)     NAME

   CO          28.011
-.26417+05   .25539+05   .58640+01   .21499-02   .42295+05   .66789+02   300.  1000.   CO
-.26417+05   .22179+05   .57638+01   .11821-02   .11103+07   .65218+02  1000.  2500.   CO
   CO2         44.011
-.94054+05   .41438+05   .95778+01   .36020-02  -.16389+06   .81997+02   300.  1000.   CO2
-.94054+05   .36573+05   .13972+02   .38449-03  -.13412+07   .79867+02  1000.  2500.   CO2
   CH4         16.043
-.17895+05   .66727+05   .56930+01   .11565-01  -.66950+05   .88496+02   300.  1000.   CH4
-.17895+05   .53270+05   .20336+02   .16707-02  -.48155+07   .82684+02  1000.  2500.   CH4
   H2O         18.016
-.57798+05   .31716+05   .68290+01   .29575-02   .27843+05   .69022+02   300.  1000.   H2O
-.57798+05   .30303+05   .99698+01   .12774-02  -.14328+07   .68463+02  1000.  2500.   H2O
   O2          32.000
 .00000      .25541+05   .67044+01   .16795-02  -.19419+05   .68908+02   300.  1000.   O2
 .00000      .23450+05   .80725+01   .50513-03  -.21319+06   .67976+02  1000.  2500.   O2
   N2          28.016
 .79000+00   .23993+05   .61391+01   .16415-02   .29727+05   .64548+02   300.  1000.   N2
 .79000+00   .22188+05   .83049+01   .23357-03  -.72806+06   .63774+02  1000.  2500.   N2
   H2           2.016
 .20000+00   .20180+05   .67559+01   .43063-03   .21903+04   .47986+02   300.  1000.   H2
 .20000+00   .21258+05   .65812+01   .82395-03  -.21635+06   .48484+02  1000.  2500.   H2
   H            1.008
 .52100+05   .13423+05   .49680+01  -.79563-08  -.65188+00   .38862+02   300.  1000.   H
 .52100+05   .13423+05   .49680+01  -.21457-08  -.38277+01   .38862+02  1000.  2500.   H
   O           16.000
 .59559+05   .13449+05   .50132+01  -.35760-04   .21105+05   .50064+02   300.  1000.   O
 .59559+05   .13517+05   .49475+01   .10904-04   .40118+05   .50094+02  1000.  2500.   O
   HO          17.008
 .94320+04   .21099+05   .64878+01   .77321-03   .41428+05   .61183+02   300.  1000.   HO
 .94320+04   .21452+05   .72179+01   .58712-03  -.50251+06   .61372+02  1000.  2500.   HO
   HO2         33.008
 .50000+04   .36387+05   .82485+01   .32199-02  -.82934+05   .81654+02   300.  1000.   HO2
 .50000+04   .32593+05   .12102+02   .54010-03  -.12571+07   .80006+02  1000.  2500.   HO2
   CH3         15.035
 .34820+05   .48677+05   .80457+01   .60835-02  -.58069+05   .81068+02   300.  1000.   CH3
 .34820+05   .42779+05   .15742+02   .12359-02  -.29064+07   .78562+02  1000.  2500.   CH3
   CH2O        30.027
-.27700+05   .54354+05   .68621+01   .80908-02  -.82595+05   .89490+02   300.  1000.   CH2O
-.27700+05   .43898+05   .17110+02   .85504-03  -.30943+07   .84938+02  1000.  2500.   CH2O
   CHO         29.019
-.29000+04   .37003+05   .74602+01   .38023-02  -.33115+05   .80992+02   300.  1000.   CHO
-.29000+04   .32424+05   .12304+02   .49109-03  -.15653+07   .79009+02  1000.  2500.   CHO
   CH2         14.027
 .92070+05   .38633+05   .68255+01   .45866-02  -.66146+05   .71042+02   300.  1000.   CH2
 .92070+05   .33805+05   .12734+02   .75955-03  -.21478+07   .68955+02  1000.  2500.   CH2
   CH          13.019
 .14200+06   .23912+05   .59808+01   .17091-02   .44673+05   .62404+02   300.  1000.   CH
 .14200+06   .23558+05   .82312+01   .70295-03  -.11995+07   .62311+02  1000.  2500.   CH
```

```
                              * KINETIC REACTION DATA *

        NUMBER OF REACTIONS= 37

  M              REACTION                     PRE EXP FACTOR  TEMP EXP      ACTIVATION       INDIVIDUAL THIRD BODY EFFIC.
                                               (MOLE-CM-S)                  (KCAL/MOLE)      NAME1      ETB1  NAME2     ETB2

  1  CH4 +     +M   --=   CH3 +H              .1500+19+ 0.      .000         100.0000                    .000              .000
  2  CH4 +HO   +    --=   CH3 +H2O            .1000+14+ 0.      .000           6.0000                    .000              .000
  3  CH4 +H    +    --=   CH3 +H2             .2000+15+ 0.      .000          11.9000                    .000              .000
  4  CH4 +O    +    --=   CH3 +HO             .2000+14+ 0.      .000           6.9000                    .000              .000
  5  CH3 +O    +    --=   CH2O+H              .3500+14+ 0.      .000           3.3000                    .000              .000
  6  CH3 +O2   +    --=   CH2O+HO             .1000+13+ 0.      .000          15.0000                    .000              .000
  7  CH2O+     +M   --=   CO  +H2             .2000+17+ 0.      .000          35.0000                    .000              .000
  8  CH2O+HO   +    --=   CHO +H2O            .2500+14+ 0.      .000           1.0000                    .000              .000
  9  CH2O+O    +    --=   CHO +HO             .3000+14+ 0.      .000            .0000                    .000              .000
 10  CH2O+H    +    --=   CHO +H2             .1700+14+ 0.      .000           3.0000                    .000              .000
 11  CHO +O2   +    --=   CO  +HO2            .3000+14+ 0.      .000            .0000                    .000              .000
 12  CHO +HO   +    --=   CO  +H2O            .1000+15+ 0.      .000            .0000                    .000              .000
 13  CHO +O    +    --=   CO  +HO             .5400+12+ 0.      .500            .0000                    .000              .000
 14  CHO +     +M   --=   CO  +H              .2000+13+ 0.      .500          28.8000                    .000              .000
 15  CO  +HO   +    --=   CO2 +H              .5500+12+ 0.      .000           1.0800                    .000              .000
 16  CO  +O    +M   --=   CO2 +               .3600+19+ 0.    -1.000           2.5000                    .000              .000
 17  HO2 +O    +    --=   O2  +HO             .2500+14+ 0.      .000            .0000                    .000              .000
 18  HO2 +HO   +    --=   O2  +H2O            .2500+14+ 0.      .000            .0000                    .000              .000
 19  HO2 +H    +    --=   HO  +HO             .2500+15+ 0.      .000           2.0000                    .000              .000
 20  HO2 +H    +    --=   O2  +H2             .2500+14+ 0.      .000            .0000                    .000              .000
 21  H   +O2   +M   --=   HO2 +               .2000+16+ 0.      .000            .8700        H2O      20.000              .000
 22  H   +O2   +    --=   HO  +O              .2200+15+ 0.      .000          16.8000                    .000              .000
 23  O   +H2   +    --=   HO  +H              .1700+14+ 0.      .000           9.4600                    .000              .000
 24  HO  +H2   +    --=   H2O +H              .2200+14+ 0.      .000           5.2000                    .000              .000
 25  HO  +HO   +    --=   H2O +O              .6000+13+ 0.      .000            .7800                    .000              .000
 26  H   +HO   +M   --=   H2O +               .7000+20+ 0.    -1.000            .0000                    .000              .000
 27  O   +H    +M   --=   HO  +               .4000+19+ 0.    -1.000            .0000                    .000              .000
 28  H   +H    +M   --=   H2  +               .2000+20+ 0.    -1.000            .0000                    .000              .000
 29  O   +O    +M   --=   O2  +               .4000+19+ 0.    -1.000            .0000                    .000              .000
 30  CH3 +HO   +    --=   CH2 +H2O            .6000+10+ 0.      .700           2.0000                    .000              .000
 31  CH2 +HO   +    --=   CH  +H2O            .5000+12+ 0.      .500           6.0000                    .000              .0C0
 32  CH2 +O2   +    --=   CH2O+O              .5000+12+ 0.      .500           7.0000                    .000              .000
 33  CH  +O2   +    --=   CHO +O              .5000+12+ 0.      .500           6.0000                    .000              .000
 34  CH2 +O    +    --=   CHO +H              .5000+12+ 0.      .500           4.0000                    .000              .000
 35  CH  +HO   +    --=   CHO +H              .5000+12+ 0.      .500          10.0000                    .000              .000
 36  CH  +O    +    --=   CO  +H              .5000+12+ 0.      .500           4.0000                    .000              .000
 37  CH2 +H    +    --=   CH  +H2             .3000+12+ 0.      .700          26.0000                    .000              .000
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           * MOLE FLUXES AT GRID POINTS(MOLE/(CM2*S)) ITERATION   6 *

           REACTION CREATION/DIFFUSION FLUX OUT/CONVECTIVE FLUX OUT


STATION NO.= 1      NODAL WIDTH= .00000    (CM)
     CH4          O2          CO2          H2O          H2          CO          CH3          CH2O
         CHO          HO2          H           O           HO          N2          CH          CH2

    .00000      .00000      .00000      .00000      .00000      .00000      .00000      .00000
        .00000      .00000      .00000      .00000      .00000      .00000      .00000      .00000

    .00000      .00000      .00000      .00000      .00000      .00000      .00000      .00000
        .00000      .00000      .00000      .00000      .00000      .00000      .00000      .00000

    .13787-03   .28930-03   .15151-11   .15151-11   .15151-11   .15151-11   .15151-11   .15151-11
        .15151-11   .15151-11   .15151-11   .15151-11   .15151-11   .10878-02   .15151-11   .15151-11

STATION NO.= 2      NODAL WIDTH= .10314-01 (CM)
     CH4          O2          CO2          H2O          H2          CO          CH3          CH2O
         CHO          HO2          H           O           HO          N2          CH          CH2

    .37527-10  -.24806-10   .61632-11   .39389-10  -.21749-10   .20125-10  -.40059-10  -.14088-10
       -.15180-11   .15571-10  -.23589-11  -.42651-11  -.33498-10   .00000     -.10687-11  -.70811-11

    .32220-05   .47140-05  -.47397-06  -.91028-05  -.62950-05  -.98698-06  -.73102-06  -.44595-07
       -.34429-14  -.71495-08  -.85542-12  -.40342-11  -.41759-10   .12569-05  -.36262-13  -.20932-10

    .13466-03   .28469-03   .47402-06   .91041-05   .62976-05   .98709-06   .73108-06   .44588-07
        .54934-15   .71672-08   .11477-13   .12843-11   .97779-11   .10866-02   .48275-12   .15368-10

STATION NO.= 3      NODAL WIDTH= .70123-02 (CM)
     CH4          O2          CO2          H2O          H2          CO          CH3          CH2O
         CHO          HO2          H           O           HO          N2          CH          CH2

    .43241-09  -.10181-09   .41563-10   .25592-09  -.21239-09   .77033-10  -.45249-09  -.68919-10
       -.40918-13   .61489-10  -.79549-10  -.20451-10  -.24604-09   .00000     -.18417-11  -.27722-10

    .67524-05   .98131-05  -.11863-05  -.17547-04  -.84499-05  -.21949-05  -.13955-05  -.86032-07
       -.48678-13  -.16626-07  -.81867-10  -.27913-10  -.32506-09   .17345-05  -.19090-11  -.67044-10

    .13114-03   .27961-03   .11866-05   .17552-04   .84559-05   .21954-05   .13954-05   .85973-07
        .48597-14   .16708-07   .31904-12   .47131-11   .47060-10   .10863-02   .51398-12   .33767-10

STATION NO.= 4      NODAL WIDTH= .46480-02 (CM)
     CH4          O2          CO2          H2O          H2          CO          CH3          CH2O
         CHO          HO2          H           O           HO          N2          CH          CH2

    .52351-08  -.56091-09   .22677-09   .15197-08  -.15504-08   .29496-09  -.53928-08  -.26125-09
       -.35146-12   .36184-09  -.26778-08  -.94727-10  -.14738-08   .00000     -.87540-11  -.97694-10
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                 * GRID INFORMATION SUMMARY TABLE *

ITERATICN=   6       NUMBER OF GRID POINTS=  25


 FLAME SPEED PAR= .39096-01        FLAME SPEED= .37049+02 CM/SEC


 GRID COORDINATES(CM)

  .00000      .12355-01   .20430-01   .26333-01   .29550-01   .31255-01   .33042-01   .34920-01
      .36900-01   .38995-01   .41215-01   .43572-01   .46077-01   .48743-01   .51581-01   .57771-01
          .64595-01   .79386-01   .11869+00   .15949+00   .24308+00   .32805+00   .49987+00   .67291+00
              .10204+01

NONDIMENSIONAL GRID INCREMENTS
  .50000+00   .30000+00   .20000+00   .10000+00   .50000-01   .50000-01   .50000-01   .50000-01
      .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .10000+00   .10000+00
          .20000+00   .50000+00   .50000+00   .10000+01   .10000+01   .20000+01   .20000+01   .40000+01
              .40000+01

TIME(SEC)

  .00000      .30979-03   .48572-03   .59680-03   .64960-03   .67511-03   .69995-03   .72409-03
      .74751-03   .77019-03   .79211-03   .81328-03   .83368-03   .85335-03   .87233-03   .90844-03
          .94261-03   .10085-02   .11703-02   .13313-02   .16524-02   .19730-02   .26141-02   .32554-02
              .45388-02

ENTHALPY(CAL/GM)

 -.58651+02  -.59301+02  -.58483+02  -.56683+02  -.54830+02  -.53498+02  -.51915+02  -.50068+02
     -.47959+02  -.45615+02  -.43083+02  -.40479+02  -.37982+02  -.35924+02  -.34837+02  -.37314+02
         -.47699+02  -.63504+02  -.63877+02  -.61844+02  -.61400+02  -.61483+02  -.62565+02  -.64171+02
             -.66432+02

TEMPERATURE(K)

 .29800+03   .34300+03   .39141+03   .45714+03   .51233+03   .54914+03   .59182+03   .64110+03
     .69775+03   .76252+03   .83616+03   .91932+03   .10125+04   .11159+04   .12289+04   .14577+04
         .16638+04   .18507+04   .19693+04   .20408+04   .20928+04   .21269+04   .21497+04   .21631+04
             .21689+04

DENSITY(GM/CM3)

 .11323-02   .97820-03   .85484-03   .72994-03   .65015-03   .60595-03   .56167-03   .51792-03
     .47530-03   .43429-03   .39544-03   .35900-03   .32533-03   .29467-03   .26719-03   .22463-03
         .19668-03   .17762-03   .16812-03   .16290-03   .15941-03   .15722-03   .15584-03   .15507-03
             .15479-03

SYSTEM MOLECULAR WEIGHT
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.27687+02   .27530+02   .27454+02   .27381+02   .27333+02   .27305+02   .27277+02   .27247+02
     .27214+02   .27174+02   .27132+02   .27081+02   .27029+02   .26981+02   .26943+02   .26869+02
          .26854+02   .26974+02   .27167+02   .27280+02   .27376+02   .27439+02   .27490+02   .27525+02
               .27549+02
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              * MOLE FRACTIONS OF  16  SPECIES *

CH4

 .91000-01  .88373-01  .85828-01  .82353-01  .79372-01  .77340-01  .74936-01  .72084-01
    .68694-01  .64657-01  .59855-01  .54163-01  .47489-01  .39829-01  .31378-01  .15224-01
       .42845-02  .25452-03  .96100-05  .39293-06  .16692-07  .70666-09  .28210-10  .98201-12
          .29459-13
O2

 .19100+00  .18683+00  .18300+00  .17784+00  .17345+00  .17047+00  .16695+00  .16281+00
    .15792+00  .15217+00  .14540+00  .13744+00  .12815+00  .11736+00  .10501+00  .78312-01
       .52274-01  .29323-01  .21833-01  .18527-01  .16169-01  .14496-01  .13257-01  .12370-01
          .11774-01
CO2

 .10000-08  .31109-03  .77665-03  .15494-02  .23188-02  .28940-02  .36109-02  .45040-02
    .56158-02  .69984-02  .87155-02  .10843-01  .13471-01  .16699-01  .20621-01  .29778-01
       .40879-01  .58695-01  .69599-01  .74487-01  .78052-01  .80603-01  .82685-01  .84187-01
          .85231-01
H2O

 .10000-08  .59751-02  .11488-01  .18537-01  .24212-01  .27914-01  .32177-01  .37084-01
    .42726-01  .49208-01  .56639-01  .65129-01  .74770-01  .85590-01  .97479-01  .12154+00
       .14219+00  .15716+00  .16289+00  .16706+00  .17065+00  .17316+00  .17496+00  .17623+00
          .17707+00
H2

 .10000-08  .41333-02  .55350-02  .67830-02  .75463-02  .79706-02  .84184-02  .88910-02
    .93903-02  .99179-02  .10476-01  .11063-01  .11677-01  .12300-01  .12894-01  .13728-01
       .13247-01  .10215-01  .82144-02  .67314-02  .51450-02  .40530-02  .31755-02  .25857-02
          .21852-02
CO

 .10000-08  .64784-03  .14370-02  .26008-02  .36521-02  .43895-02  .52746-02  .63366-02
    .76102-02  .91362-02  .10963-01  .13145-01  .15741-01  .18808-01  .22362-01  .29891-01
       .35085-01  .28382-01  .19352-01  .15046-01  .11838-01  .95421-02  .76412-02  .62707-02
          .53151-02
CH3

 .10000-08  .47981-03  .91333-03  .14622-02  .19017-02  .21892-02  .25237-02  .29171-02
    .33859-02  .39503-02  .46309-02  .54389-02  .63567-02  .73013-02  .80758-02  .80184-02
       .47099-02  .55042-03  .30214-04  .14242-05  .58115-07  .22238-08  .78075-10  .24293-11
          .66386-13
CH2O

 .10000-08  .29263-04  .56272-04  .90829-04  .11871-03  .13695-03  .15803-03  .18246-03
    .21090-03  .24424-03  .28348-03  .32917-03  .37957-03  .42683-03  .45322-03  .37229-03
       .17888-03  .15607-04  .43212-06  .11345-07  .30015-09  .31079-10  .15651-10  .10375-10
          .74411-11
CHO

 .10000-08  .36683-12  .32464-11  .30257-10  .15202-09  .39252-09  .10238-08  .27184-08
    .72564-08  .19255-07  .50811-07  .13455-06  .35838-06  .94264-06  .23387-05  .85425-05
       .13432-04  .30085-05  .16394-06  .38654-07  .22418-07  .15121-07  .10347-07  .75794-08
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                .59146-08
HO2

  .10000-08   .47079-05   .10945-04   .20562-04   .29495-04   .35736-04   .42969-04   .50918-04
       .58967-04   .66356-04   .72710-04   .78477-04   .84752-04   .91973-04   .97826-04   .85178-04
            .42956-04   .79940-05   .37320-05   .26307-05   .18284-05   .13024-05   .93536-06   .71116-06
                .57740-06
H

  .10000-08   .70929-11   .20880-11   .89551-08   .16090-06   .69889-06   .22599-05   .62295-05
       .15001-04   .32257-04   .63416-04   .11681-03   .20640-03   .35666-03   .60785-03   .15635-02
            .32148-02   .51455-02   .37082-02   .23999-02   .14229-02   .91117-03   .59159-03   .41462-03
                .31251-03
O

  .10000-08   .85966-09   .31741-08   .13810-07   .39901-07   .74684-07   .14429-06   .29820-06
       .66815-06   .16057-05   .40288-05   .10240-04   .25757-04   .63167-04   .14933-03   .61045-03
            .17030-02   .31391-02   .24175-02   .16920-02   .11159-02   .78146-03   .55711-03   .42205-03
                .33906-03
HO

  .10000-08   .64702-08   .30994-07   .15735-06   .54226-06   .11274-05   .22958-05   .46463-05
       .92588-05   .18081-04   .34903-04   .67768-04   .13391-03   .26771-03   .52851-03   .16294-02
            .36338-02   .66267-02   .69743-02   .64134-02   .55531-02   .48407-02   .41990-02   .37153-02
                .33569-02
N2

  .71800+00   .71313+00   .71093+00   .70888+00   .70759+00   .70688+00   .70613+00   .70535+00
       .70453+00   .70369+00   .70286+00   .70206+00   .70134+00   .70073+00   .70020+00   .69913+00
            .69853+00   .70047+00   .70496+00   .70764+00   .71005+00   .71161+00   .71293+00   .71381+00
                .71442+00
CH

  .10000-08   .36147-09   .50144-09   .16755-08   .51694-08   .10978-07   .11259-07   .53688-08
       .18615-08   .16563-08   .81259-11   .18286-08   .11585-07   .37156-07   .13354-06   .96964-06
            .35853-05   .27551-05   .28749-06   .15938-07   .60085-09   .19839-10   .58036-12   .15306-13
                .36359-15
CH2

  .10000-08   .10097-07   .22125-07   .47679-07   .86381-07   .12554-06   .18763-06   .29043-06
       .46650-06   .77763-06   .13482-05   .24357-05   .45714-05   .87266-05   .16276-04   .42575-04
            .58899-04   .15527-04   .10828-05   .52021-07   .19583-08   .68142-10   .21571-11   .61332-13
                .15550-14
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                  * NET FORWARD KINETIC FRODUCTION RATES(MOLE/(CC*SEC)) FOR    37  REACTIONS *

REACTICN NUMBER   1
  .00000     -.30294-08  -.47914-07  -.97471-06  -.83038-05  -.24132-04  -.51469-04  -.92254-04
      -.14341-03  -.19908-03  -.25433-03  -.30764-03  -.36081-03  -.41591-03  -.46899-03  -.51210-03
          -.33646-03  -.39670-04  -.12096-05  -.31651-07  -.67137-09  -.14302-10  -.26088-12  -.38552-14
              -.37096-16
REACTICN NUMBER   2
  .00000      .10720-08   .11402-07   .12378-06   .66807-06   .17506-05   .44233-05   .10864-04
       .25529-04   .56723-04   .11935-03   .24003-03   .46241-03   .83771-03   .13692-02   .20950-02
           .12478-02   .12107-03   .39867-05   .12033-06   .36232-08   .11642-09   .36633-11   .10538-12
               .27407-14
REACTICN NUMBER   3
  .00000     -.17530-08  -.25821-07  -.28345-06  -.11756-05  -.24636-05  -.48867-05  -,86012-05
      -.11599-04  -.48812-05   .36800-04   .16818-03   .48577-03   .11231-02   .21800-02   .44098-02
           .32884-02   .36817-03   .93322-05   .20893-06   .44617-08   .10775-09   .25795-11   .59353-13
               .12941-14
REACTICN NUMBER   4
  .00000      .71778-10   .66724-09   .72076-08   .35958-07   .90596-07   .23137-06   .62120-06
       .17658-05   .51944-05   .15204-04   .42545-04   .11009-03   .25648-03   .52357-03   .11358-02
           .89413-03   .90943-04   .22156-05   .51238-07   .11815-08   .30579-10   .79163-12   .19494-13
               .45043-15
REACTICN NUMBER   5
  .00000      .14072-09   .13701-08   .12836-07   .57024-07   .13472-06   .32321-06   .81992-06
       .22291-05   .64178-05   .19027-04   .56249-04   .16098-03   .43449-03   .10739-02   .38283-02
           .55438-02   .10676-02   .42078-04   .13314-05   .34770-07   .91362-09   .22572-10   .52800-12
               .11552-13
REACTICN NUMBER   6
  .00000      .31091-10   .67734-09   .12375-07   .74055-07   .19588-06   .51322-06   .13147-05
       .32517-05   .76764-05   .17106-04   .35571-04   .68062-04   .11761-03   .17880-03   .24680-03
           .14106-03   .11821-04   .54556-06   .23241-07   .86285-09   .30367-10   .99109-12   .29045-13
               .75840-15
REACTICN NUMBER   7
  .00000      .36291-19   .30753-16   .23551-13   .15575-11   .15683-10   .15753-09   .15284-08
       .13889-07   .11506-06   .84974-06   .54917-05   .30466-04   .14137-03   .52886-03   .29298-02
           .48271-02   .99210-03   .43022-04   .14309-05   .38925-07   .99202-09  -.29271-11  -.12374-10
              -.56895-11
REACTICN NUMBER   8
  .00000      .13647-08   .11597-07   .84009-07   .33982-06   .75853-06   .16405-05   .34887-05
       .72330-05   .14567-04   .28776-04   .56684-04   .11198-03   .21699-03   .39081-03   .74982-03
           .64356-03   .85328-04   .22325-05   .50600-07   .10809-08   .74476-10   .24395-10   .10716-10
               .47931-11
REACTICN NUMBER   9
  .00000      .93330-09   .50434-08   .25878-07   .78101-07   .14878-06   .28727-06   .58664-06
       .12869-05   .30044-05   .72795-05   .17776-04   .42501-04   .96475-04   .19961-03   .47616-03
           .48982-03   .63666-04   .11991-05   .20502-07   .33161-09   .18309-10   .49211-11   .18489-11
               .73505-12
REACTICN NUMBER  10
  .00000      .57860-13   .40827-11   .40161-09   .97376-08   .51267-07   .20055-06   .66168-06
       .18831-05   .47199-05   .10665-04   .22222-04   .43419-04   .79738-04   .13471-03   .24523-03
           .21139-03   .26150-04   .48408-06   .78615-08   .11639-09   .59289-11   .14597-11   .50913-12
               .19013-12
REACTICN NUMBER  11
  .00000      .25489-08   .16913-07   .11226-06   .43805-06   .97702-06   .21541-05   .47671-05
       .10456-04   .22405-04   .46952-04   .97143-04   .19863-03   .39327-03   .71845-03   .13856-02
```

```
     * RATIO OF FORWARD TO BACKWARD KINETIC PRODUCTION RATES FOR  37  REACTIONS *


REACTICN NUMBER   1
  .00000      .00000      .00000      .13489-33   .17235-29   .36487-27   .10598-24   .33509-22
        .10180-19   .26517-17   .53511-15   .76795-13   .73109-11   .43809-09   .16003-07   .31324-05
              .74136-04   .64123-03   .35944-02   .12694-01   .43228-01   .11340+00   .26039+00   .48648+00
                    .75760+00
REACTICN NUMBER   2
  .00000      .17341+07   .16137+06   .21512+05   .77554+04   .46439+04   .27009+04   .15648+04
        .90318+03   .52068+03   .30399+03   .18353+03   .11627+03   .77143+02   .52680+02   .25189+02
              .12302+02   .65539+01   .35798+01   .24316+01   .19551+01   .17521+01   .16462+01   .15822+01
                    .15471+01
REACTICN NUMBER   3
  .00000      .24917-05   .30322-04   .83690-03   .10272-01   .38071-01   .10556+00   .24802+00
        .50298+00   .89420+00   .14185+01   .20466+01   .27387+01   .34627+01   .41875+01   .52080+01
              .54225+01   .57427+01   .35312+01   .24121+01   .19428+01   .17435+01   .16408+01   .15786+01
                    .15449+01
REACTION NUMBER   4
  .00000      .22188+02   .14219+02   .12351+02   .10956+02   .10340+02   .10182+02   .10683+02
        .12139+02   .14728+02   .18285+02   .22032+02   .24753+02   .25630+02   .24793+02   .19257+02
              .12844+02   .70550+01   .36649+01   .24583+01   .19692+01   .17610+01   .16520+01   .15858+01
                    .15493+01
REACTICN NUMBER   5
  .00000      .60909-07   .64333-06   .66405-05   .19007+30   .82461+27   .48062+25   .36917+23
        .39531+21   .60577+19   .13250+18   .40666+16   .17197+15   .99384+13   .79021+12   .17118+11
              .14472+10   .26707+09   .18172+09   .18961+09   .21279+09   .65815+08   .42358+07   .19433+06
                    .75607+04
REACTICN NUMBER   6
  .00000      .13457-07   .31804-06   .63212+33   .32205+30   .45487+28   .64543+26   .95364+24
        .15547+23   .29341+21   .65756+19   .17633+18   .56976+16   .22695+15   .11629+14   .10877+12
              .40253+10   .32222+09   .18782+09   .19242+09   .21532+09   .66517+08   .42742+07   .19569+06
                    .75975+04
REACTICN NUMBER   7
  .00000      .93219+06   .80741+06   .82757+06   .88708+06   .93498+06   .99461+06   .10662+07
        .11495+07   .12441+07   .13478+07   .14548+07   .15491+07   .15962+07   .15446+07   .10769+07
              .51239+06   .77132+05   .40366+04   .16940+03   .75424+01   .12386+01   .99894+00   .99356+00
                    .99593+00
REACTICN NUMBER   8
  .00000      .37154+30   .92014+26   .19846+23   .89565+20   .43909+19   .20810+18   .99175+16
        .49595+15   .27224+14   .17003+13   .12419+12   .10805+11   .11279+10   .14136+09   .49325+07
              .45015+06   .76312+05   .19221+05   .12947+04   .38240+02   .42538+01   .24065+01   .17940+01
                    .14428+01
REACTICN NUMBER   9
  .00000      .47540+25   .81078+22   .11395+20   .12653+18   .97766+16   .78450+15   .67707+14
        .66655+13   .77004+12   .10227+12   .14908+11   .23004+10   .37475+09   .66528+08   .37710+07
              .46999+06   .82147+05   .19678+05   .13090+04   .38515+02   .42753+01   .24150+01   .17982+01
                    .14449+01
REACTICN NUMBER  10
  .00000      .53386+18   .17290+17   .77209+15   .11862+15   .35997+14   .81335+13   .15719+13
        .27619+12   .46754+11   .79341+10   .13848+10   .25451+09   .50629+08   .11237+08   .10198+07
              .19842+06   .66867+05   .18960+05   .12844+04   .37998+02   .42328+01   .23987+01   .17900+01
                    .14408+01
REACTICN NUMBER  11
  .00000      .82338+07   .47777+06   .41331+05   .11159+05   .57907+04   .30130+04   .16351+04
        .93648+03   .56915+03   .37100+03   .26098+03   .19638+03   .15483+03   .12533+03   .87907+02
```

```
               * KINETIC CONTRIBUTIONS TO INDIVIDUAL SPECIES(MOLE/(CC*SEC)) REACTION/CONTRIBUTION  *
      GRID POINT   2
     CH4      ( 1/ .303-08),  ( 2/-.107-08),  ( 3/ .175-08),  ( 4/-.718-10),  (
     O2       ( 6/-.311-10),  (11/-.255-08),  (17/ .125-09),  (18/ .952-09),  (20/ .112-11),  (21/-.394-10),
                 (22/ .848-13),  (29/ .371-15),  (32/-.760-09),  (33/-.104-09),  (
     CO2      (15/ .591-09),  (16/ .655-11),  (
     H2O      ( 2/ .107-08),  ( 8/ .136-08),  (12/ .292-15),  (18/ .952-09),  (24/ .357-09),  (25/ .992-13),
                 (26/ .442-15),  (30/ .737-10),  (31/ .113-15),  (
     H2       ( 3/-.175-08),  ( 7/ .363-19),  (10/ .579-13),  (20/ .112-11),  (23/-.698-13),  (24/-.357-09),
                 (28/ .148-18),  (37/-.373-26),  (
     CO       ( 7/ .363-19),  (11/ .255-08),  (12/ .292-15),  (13/ .383-17),  (14/-.424-14),  (15/-.591-09),
                 (16/-.655-11),  (36/ .880-17),  (
     CH3      ( 1/-.303-08),  ( 2/ .107-08),  ( 3/-.175-08),  ( 4/ .718-10),  ( 5/-.141-09),  ( 6/-.311-10),
                 (30/-.737-10),  (
     CH2O     ( 5/ .141-09),  ( 6/ .311-10),  ( 7/-.363-19),  ( 8/-.136-08),  ( 9/-.933-09),  (10/-.579-13),
                 (32/ .760-09),  (
     CHO      ( 8/ .136-08),  ( 9/ .933-09),  (10/ .579-13),  (11/-.255-08),  (12/-.292-15),  (13/-.383-17),
                 (14/ .424-14),  (33/ .104-09),  (34/ .280-15),  (35/ .100-19),  (
     HO2      (11/ .255-08),  (17/-.125-09),  (18/-.952-09),  (19/-.593-12),  (20/-.112-11),  (21/ .394-10),
                 (
     H        ( 1/-.303-08),  ( 3/ .175-08),  ( 5/ .141-09),  (10/-.579-13),  (14/-.424-14),  (15/ .591-09),
                 (19/-.593-12),  (20/-.112-11),  (21/-.394-10),  (22/ .848-13),  (23/ .698-13),  (24/ .357-09),
                       (26/-.442-15)   (27/-.332-17)   (28/-.296-18)   (34/ .280-15)   (35/ .100-19)   (36/ .880-17)
37/ .373-26)   (
     O        ( 4/-.718-10),  ( 5/-.141-09),  ( 9/-.933-09),  (13/-.383-17),  (16/-.655-11),  (17/-.125-09),
                 (22/-.848-13),  (23/-.698-13),  (25/ .992-13),  (27/-.332-17),  (29/-.742-15),  (32/ .760-09),
                       (33/ .104-09)   (34/-.280-15)   (36/-.880-17)   (
     HO       ( 2/-.107-08),  ( 4/ .718-10),  ( 6/ .311-10),  ( 8/-.136-08),  ( 9/ .933-09),  (12/-.292-15),
                 (13/ .383-17),  (15/-.591-09),  (17/ .125-09),  (18/-.952-09),  (19/ .119-11),  (22/-.848-13),
                       (23/ .698-13)   (24/-.357-09)   (25/-.198-12)   (26/-.442-15)   (27/ .332-17)   (30/-.737-10)
31/-.113-15)   (35/-.100-19)   (
     CH       (31/ .113-15),  (33/-.104-09),  (35/-.100-19),  (36/-.880-17),  (37/-.373-26),  (
     CH2      (30/ .737-10),  (31/-.113-15),  (32/-.760-09),  (34/-.280-15),  (37/ .373-26),  (

      GRID POINT   3
     CH4      ( 1/ .479-07),  ( 2/-.114-07),  ( 3/ .258-07),  ( 4/-.667-09),  (
     O2       ( 6/-.677-09),  (11/-.169-07),  (17/ .817-09),  (18/ .816-08),  (20/ .553-10),  (21/-.926-09),
                 (22/ .112-11),  (29/ .293-14),  (32/-.477-08),  (33/-.263-09),  (
     CO2      (15/ .588-08),  (16/ .493-10),  (
     H2O      ( 2/ .114-07),  ( 8/ .116-07),  (12/ .949-14),  (18/ .816-08),  (24/ .453-08),  (25/ .202-11),
                 (26/ .347-13),  (30/ .815-09),  (31/ .290-14),  (
     H2       ( 3/-.258-07),  ( 7/ .308-16),  (10/ .408-11),  (20/ .553-10),  (23/-.146-11),  (24/-.453-08),
                 (28/ .672-16),  (37/-.733-24),  (
     CO       ( 7/ .308-16),  (11/ .169-07),  (12/ .949-14),  (13/ .102-15),  (14/-.214-12),  (15/-.588-08),
                 (16/-.493-10),  (36/ .580-16),  (
     CH3      ( 1/-.479-07),  ( 2/ .114-07),  ( 3/-.258-07),  ( 4/ .667-09),  ( 5/-.137-08),  ( 6/-.677-09),
                 (30/-.815-09),  (
     CH2O     ( 5/ .137-08),  ( 6/ .677-09),  ( 7/-.308-16),  ( 8/-.116-07),  ( 9/-.504-08),  (10/-.408-11),
                 (32/ .477-08),  (
     CHO      ( 8/ .116-07),  ( 9/ .504-08),  (10/ .408-11),  (11/-.169-07),  (12/-.949-14),  (13/-.102-15),
                 (14/ .214-12),  (33/ .263-09),  (34/ .381-14),  (35/ .258-18),  (
     HO2      (11/ .169-07),  (17/-.817-09),  (18/-.816-08),  (19/-.422-10),  (20/-.553-10),  (21/ .926-09),
                 (
     H        ( 1/-.479-07),  ( 3/ .258-07),  ( 5/ .137-08),  (10/-.408-11),  (14/-.214-12),  (15/ .588-08),
                 (19/-.422-10),  (20/-.553-10),  (21/-.926-09),  (22/ .112-11),  (23/ .146-11),  (24/ .453-08),
                       (26/-.347-13)   (27/-.198-15)   (28/-.134-15)   (34/ .381-14)   (35/ .258-18)   (36/ .580-16)
```

solution can be found. Besides giving valuable information on flame speed, free flame predictions can be used as good enthalpy and species first guesses for attached flame calculations. Thus, it is advantageous to run a free flame calculation prior to running an attached flame calculation at the same reactant initial conditions.

This free flame sample case consists of an unconfined, atmospheric pressure, methane/air flame which has an initial methane concentration of 9.1 percent and an initial temperature of 298°K. The nonunity Lewis number option and radiation heat loss, are specified for this case. Curve fit thermochemical data is used in this calculation. Curve fit data, though slightly less accurate than tabular data, gives precise property derivatives which improves solution convergence characteristics.

In order to align the solution grid in an efficient manner, the code makes use of an arbitrary constraint condition. Typically the finer grid zone is aligned with the flame zone by this process. The flame zone is arbitrarily identified by the concentration of some species or a specified temperature. For this case the constraint is applied to the methane concentration which monotonically decreases through the flame. A value roughly two thirds of the initial concentration is chosen as the contraint value. Typically, a value of the constraint variable midway between its preflame and postflame values should be selected. This provides the best numerical stability and assures adequate definition of the flame in the zone of steepest gradients. The constraint condition is applied to the 12th grid point, which is roughly one half the total number of grid points specified. As indicated on the input listing, the grid spacings surrounding the constraint location are small. Further from the constraint grid point, where gradients diminish, the grid spacings can be increased without adversely affecting gradient definition and solution accuracy. Therefore, as shown on the input, grid spacings are increased away from the constraint grid point.

Two important flame problem parameters are APR and BP the "time scale" and "diffusion" parameters respectively. Utilizing the development given in Sections 3.1.1 and 4.1.1 the nondimensional BP parameter divided by σ_n can be written as:

$$\frac{BP}{\sigma_n} = \frac{\tilde{D}\,\rho A T^{1.659}}{\dot{m}\ ds_n} = \frac{.172 \times 10^{-4}\ T^{1.659}}{P\ ds_n\ U}$$

One way to characterize BP is to note that BP/σ_n represents the ratio of the diffusion to the convection contribution to the conservation equations. Values of the order of 1.0 should be appropriate when these phenomena contribute equally to the physical events. Of course, σ_n the nondimensional grid spacing, varies through the flame and hence BP/σ_n also varies through the flame. The objective in selecting values for BP and σ_n is to adequately cover with grid points all property gradients in the flame. Thus, the initial selection of BP or σ_n might be revised once a solution is obtained and gradient definition is seen to be inadequate.

To estimate initial values for BP and σ_n, the following approach can be taken. For example, atmospheric CH_4/air experiments indicate a flame zone thickness of the order of .1 cm. Breaking this zone into 25 increments yields a Δs_n (nee ds) of .004 cm in the flame zone. In the flame zone a mean temperature is in the range of 1200°K and we expect a flame speed of 30 cm/sec. These lead to a value of BP/σ_n from the above equation of greater than 4. If the arbitrary values of σ_n in the flame zone have been selected as .05 (down from 1.0 in the pre- and postflame zones) then a good value for BP will be on the order of 0.25. This is the value applied in the calculation. It should be noted that if the initial pressure or temperature is altered, the form of BP is such that it is not very sensitive to these changes. Therefore, flame calculations at conditions in the vicinity of this sample problem can use the value of BP applied in this case without serious problems. The criteria for whether a good value of BP and σ_n distribution has been selected for the problem is that, in the final answer, the physical grid should cover the flame sufficiently well such that gradients are well defined. If definition is not adequate, either BP should be increased and/or σ_n decreased until gradient definition is adequate.

Once BP has been fixed, APR is estimated by applying expressions 35 and 36 in Section 4.1.1. Since unburnt gas velocity and density can typically be estimated, expressions 35 and 36 are used at the first grid station. The value of APR is then given by:

$$APR = \frac{\tilde{D}}{BP(\rho_1 U_1)^2} = \frac{0.172 \cdot 10^{-4}}{P \cdot BP \cdot (\rho_1 U_1)^2}$$

where the best estimates of ρ_1 and U_1 are substituted into the above. APR is continuously updated during the calculation and the input value only represents a first guess. Further, if punched card first guesses are used from a previous calculation, as in this sample problem, then the APR value initially input is superseded by the punched card input from the prior run.

The cross sectional area change for this free flame is expected to be on the order of 10 percent and the distribution is unknown. Therefore, the flame relative area parameter, AP(N), is set equal to one over the entire grid. The grid spacing, σ_n or DS(N) distribution, is a very important parameter and determines how well the gradients through the flame are defined. The 25 grid spacings are distributed such that initially, where the temperature is low and reactions slow, moderate sized increments are applied. Through the "flame zone", where the grid constraint is applied and the relatively fast reactions are kinetically controlled, small increments are used to define the gradients. Finally, downstream of the flame the increments are made large since concentrations are slowly changing in this region. If the equilibrium state of the products are of interest a single very large step can be added to the end of the calculation. Of course, in this case radiation heat loss is active and the final equilibrium state will reflect this energy loss.

The species names and initial concentrations input are straightforward. However, the diffusion factor input requires some description. The quantities input are the inverses of the diffusion factors described in Section 3.1.1. These quantities are all referenced to molecular oxygen, and a tabulation of values for the carbon, hydrogen, nitrogen and oxygen system is given in Reference 3. In the absence of such data a good estimate for $1/F_i$ can be obtained using the expression (Appendix A):

$$\frac{1}{F_i} = \left(\frac{M_i}{26}\right)^{-0.461}$$

As indicated previously, the reference diffusion coefficient value for O_2 has been incorporated into the code. It might be noted that all D_{ij} can be increased by a factor by multiplying all $1/F_i$ by the square root of that factor. Thus, diffusion can be either increased or decreased for all species by increasing or decreasing all $1/F_i$ uniformly. This will result in a corresponding increase or decrease in thermal conductivity and viscosity.

The kinetic reaction data given on the listing is straightforward and needs no explanation. The punched card first guess data, which appears last on the input listing, was obtained from a prior run. This data supersedes species concentration guesses obtained from a linear interpolation between the previously input initial and final species concentrations.

Selected sections of output for this flame problem are presented to illustrate the type of output to be expected. The first two pages list the input data along with descriptive headings. The third page of output lists the thermochemical data to be used in the calculation. This curve fit data was obtained from the storage device denoted Unit 11. Following the listing of reaction data is the first guess species concentration data. This data is scaled to the present problem by the ratio of the current nondimensional grid spacings, σ_n or DS (N) to those input on the prior run punched card deck. For this problem the grid spacing distribution from the prior run and the current calculation are the same and the scaling is one to one.

The chemistry solution output gives the properties at each grid point. These properties are functions of the initially guessed downstream conditions and have a physical meaning only when the solution is converged. The number of iterations associated with the solution at each grid point indicates the difficulty in converging to a solution. Initially, the number of iterations are high because the properties are changing from the unreacted initial condition to a partially reacted state over a large step size. Away from the initial grid point the roughly constant number of iterations for each point indicate that the grid spacing distribution is reasonable. A single point with a large number of iterations indicates that too large a step has been taken. One test of the adequacy of the grid is to plot the species concentration as a function of distance and determine if concentration gradients have been adequately defined.

The predictor/corrector output indicates if the solution is converged. If the species concentrations in the first three lines of output are close to those in the following three lines, then the solution is converged. This also holds true for the last three items output, which are the enthalpy, temperature and enthalpy tilda (mixture enthalpy weighted by the diffusion factors). The last line of output gives the flame speed parameter, it's current correction, the maximum error in concentration, enthalpy, temperature or enthalpy tilda and the scale factor applied to the corrections to the solution estimates. A converged solution will exhibit a small flame speed parameter correction relative to the magnitude of the flame speed parameter. Also, the damping will be one, indicating full linear corrections are being made to the variables. At convergence the maximum variable error will be below 0.001, which is the code built in relative error criteria.

Prior to the condensed output for the final iteration appears the individual species reaction creation, diffusion and convective flux output for each grid point. This output is useful in assessing whether reaction or diffusion is controlling the species concentrations at a grid point.

The species equation at each grid point can be constructed from this output by taking the convective and diffusion flux output at the grid point upstream from the point of interest and adding to it the reaction creation and subtracting from it the convective and diffusion flux output at the point of interest. If the solution is converged, this equation will have a very small error. For nonconverged solutions this is not the case and the flux output is not physically meaningful.

The grid information summary table gives all of the important properties along the grid. In addition, forward kinetic reaction rate and the ratio of forward to backward kinetic reaction rate information is output at each grid point. This information is useful in assessing where each kinetic reaction becomes active and also whether that reaction approaches equilibrium along the grid. Following this, the kinetic reaction rate contribution to each species at all grid points is output. This information is useful in assessing the impact of reactions on the species concentrations along the grid. If the contribution of the reaction is not important relative to other reactions, that reaction can be removed from the data set without causing serious error. Proceeding in this manner, the dominant reactions and reaction paths can be determined using this output. This feature is very useful in testing proposed reaction mechanisms.

7.2 Sample Case 2 - Methane/Air Flame Attached to a Flameholder

This sample case demonstrates the PROF flameholder and assigned mass flowrate option. The conditions for this sample case are the same as in case 1 except that the mass rate, and hence the unreacted gas velocity, is assigned along with flameholder heat and species losses. For this case it is assumed that sufficient cooling is provided to the flameholder to maintain the gas temperature adjacent to the flameholder at 298°K. Specifying the mass flowrate then defines the heat and reactive species losses to the flameholder.

As mentioned in Section 7.1, an assigned mass rate with flameholder calculation should use a converged free flame calculation as the first guess. The results of the free flame calculation provide reasonable enthalpy and species concentration guesses for the flameholder calculation and gives the flame speed for the chemical mechanism input. Flame speed is an important parameter to know since the assigned flame speed or mass flowrate must always be smaller than the free flame speed. Values larger than the flame speed will cause flame blow-off. For this sample case, the assigned flame speed represents a velocity roughly 73 percent of the free flame speed.

SAMPLE PROBLEM 7.2

```
 1.    CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.952
 2.    16  3 16 25  8  3  1  1 -3  1  1  1 12  2  1  1
 3.   .03         .25        1.0        298.       .002       298.
 4.   1.          1.         1.         1.         1.         1.
 5.   1.          1.         1.         1.         1.         1.         1.         1.
 6.   1.          1.         1.         1.         1.         1.         1.         1.
 7.   1.          1.         1.         1.         1.         1.         1.         1.
 8.    .05        .05        .05        .05        1.         1.         1.         1.
 9.    .05        .05         .05        .05       .05        .05        .05        .05
10.     .2        .5         .5         1.0        .05        .05        .1         .1
11.    4.0                                         1.0        2.0        2.0        4.0
12.   CH4         .091                 1.-31.0523
13.   O2          .191                 1.-31.0468
14.   CO2                1.-9.1            .8
15.   H2O                1.-9.06         1.2980
16.   H2                 1.-9          1.-33.5333
17.   CO                 1.-9          1.-3 .9830
18.   CH3                1.-9          1.-31.3257
19.   CH2O               1.-9          1.-31.2980
20.   CHO                1.-9          1.-3 .9604
21.   HO2                1.-9          1.-3 .9016
22.   H                  1.-9          1.-35.1557
23.   O                  1.-9          1.-31.4158
24.   HO                 1.-9          1.-31.3475
25.   N2          .718        .718         .9732
26.   CH                 1.-9          1.-31.43
27.   CH2                1.-9          1.-31.37
28.   END
29.    37
30.   CH4         M    CH3  H          1.50+18         0.   100.0
31.   CH4  HO          CH3  H2O        1.00+13   0.0    6.000
32.   CH4  H           CH3  H2         2.00+14   0.0   11.900
33.   CH4  O           CH3  HO         2.00+13   0.0    6.900
34.   CH3  O           CH2O H          3.50+13   0.0    3.300
35.   CH3  O2          CH2O HO         1.00+12   0.0   15.000
36.   CH2O        M    CO   H2         2.00+16   0.0   35.000
37.   CH2O HO          CHO  H2O        2.50+13   0.0    1.000
38.   CH2O O           CHO  HO         3.00+13   0.0    0.
39.   CH2O H           CHO  H2         1.70+13   0.0    3.000
40.   CHO  O2          CO   HO2        3.00+13   0.0    0.
41.   CHO  HO          CO   H2O        1.00+14   0.0    0.
42.   CHO  O           CO   HO         5.40+11   0.5    0.
43.   CHO         M    CO   H          2.00+12   0.5   28.800
44.   CO   HO          CO2  H          5.50+11   0.0    1.080
45.   CO   O      M    CO2             3.60+18  -1.0    2.500
46.   HO2  O           O2   HO         2.50+13   0.0    0.
47.   HO2  HO          O2   H2O        2.50+13   0.0    0.
48.   HO2  H           HO   HO         2.50+14   0.0    2.000
49.   HO2  H           O2   H2         2.50+13   0.0     .000
50.   H    O2     M    HO2             2.00+15   0.0     .870  H2O  20.
51.   H    O2          HO   O          2.20+14   0.0   16.800
52.   O    H2          HO   H          1.70+13   0.0    9.460
53.   HO   H2          H2O  H          2.20+13   0.0    5.200
54.   HO   HO          H2O  O          6.00+12   0.0     .780
```

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 55.    H    HO   M    H2O                 7.00+19   -1.0      0.
 56.    O    H    M    HO                  4.00+18   -1.0      0.
 57.    H    H    M    H2                  2.00+19   -1.0      0.
 58.    O    O    M    O2                  4.00+18   -1.0      0.
 59.    CH3  HO        CH2  H2O            6.00+09         .7        2.0
 60.    CH2  HO        CH   H2O            5.00+11         .5        6.0
 61.    CH2  O2        CH2O O              5.00+11         .5        7.
 62.    CH   O2        CHO  O              5.00+11         .5        6.0
 63.    CH2  O         CHO  H              5.00+11      .5       4.0
 64.    CH   HO        CHO  H              5.00+11      .5      10.0
 65.    CH   O         CO   H              5.00+11      .5       4.0
 66.    CH2  H         CH   H2             3.00+11      .7       26.0
 67.     CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.752
 68.     25 16 .40331-01 .25000+00
 69.     .05     .05     .05     .05     .05     .05     .05     .05     .05     .05
 70.    .5000-01.5000-01.5000-01.5000-01.1000+00.1000+00.2000+00.5000+00.5000+00.1000+01
 71.    .1000+01.2000+01.2000+01.4000+01.4000+01
 72.    -.604+02-.604+02-.594+02-.580+02-.569+02-.555+02-.539+02-.519+02-.497+02-.472+02
 73.    -.446+02-.419+02-.396+02-.381+02-.400+02-.497+02-.639+02-.635+02-.609+02-.599+02
 74.    -.591+02-.589+02-.588+02-.587+02
 75.    .3211-02.3130-02.3018-02.2920-02.2850-02.2765-02.2663-02.2540-02.2391-02.2213-02
 76.    .2000-02.1749-02.1459-02.1139-02.5332-03.1403-03.8115-05.3037-06.1238-07.5227-09
 77.    .2185-10.8520-12.2843-13.7919-15
 78.    .6779-02.6655-02.6487-02.6341-02.6239-02.6116-02.5970-02.5797-02.5590-02.5345-02
 79.    .5053-02.4709-02.4305-02.3840-02.2837-02.1871-02.1065-02.7948-03.6733-03.5866-03
 80.    .5256-03.4812-03.4503-03.4309-03
 81.    .1153-04.2890-04.5796-04.8712-04.1090-03.1363-03.1705-03.2131-03.2661-03.3322-03
 82.    .4140-03.5151-03.6389-03.7894-03.1141-02.1560-02.2204-02.2575-02.2738-02.2856-02
 83.    .2941-02.3009-02.3056-02.3087-02
 84.    .2189-03.4226-03.6849-03.8977-03.1037-02.1197-02.1383-02.1597-02.1843-02.2126-02
 85.    .2449-02.2815-02.3225-02.3675-02.4585-02.5341-02.5840-02.6004-02.6131-02.6239-02
 86.    .6314-02.6365-02.6401-02.6422-02
 87.    .1495-03.2009-03.2473-03.2760-03.2920-03.3088-03.3267-03.3456-03.3656-03.3868-03
 88.    .4091-03.4324-03.4558-03.4780-03.5083-03.4855-03.3734-03.2992-03.2429-03.1850-03
 89.    .1457-03.1147-03.9449-04.8167-04
 90.    .2435-04.5410-04.9801-04.1376-03.1653-03.1984-03.2383-03.2861-03.3435-03.4122-03
 91.    .4944-03.5922-03.7075-03.8410-03.1123-02.1304-02.1030-02.6998-03.5438-03.4271-03
 92.    .3444-03.2772-03.2303-03.1999-03
 93.    .1134-04.2196-04.3609-04.4849-04.5762-04.6921-04.8393-04.1024-03.1251-03.1528-03
 94.    .1857-03.2229-03.2609-03.2919-03.2890-03.1606-03.1801-04.9666-06.4494-07.1811-08
 95.    .6829-10.2345-11.7027-13.1799-14
 96.    .1033-05.2046-05.3443-05.4609-05.5367-05.6217-05.7159-05.8200-05.9371-05.1072-04
 97.    .1230-04.1406-04.1572-04.1659-04.1329-04.6032-05.4928-06.1324-07.3431-09.9178-11
 98.    .1066-11.5619-12.3825-12.2874-12
 99.    .1468-11.9261-11.3293-10.6421-10.5894-10.2805-10.2149-10.1386-09.5622-09.1731-08
100.    .4844-08.1327-07.3565-07.8995-07.3312-06.4929-06.9734-07.5350-08.1360-08.7982-09
101.    .5414-09.3769-09.2856-09.2354-09
102.    .2175-06.7213-06.1661-05.2430-05.2801-05.3070-05.3202-05.3207-05.3136-05.3064-05
103.    .3065-05.3187-05.3411-05.3608-05.3064-05.1462-05.2783-06.1340-06.9411-07.6491-07
104.    .4599-07.3301-07.2529-07.2093-07
105.    .4782-11.3798-10.3956-09.2107-08.4409-08.7727-08.1206-07.1420-06.9069-06.2184-05
106.    .4276-05.7723-05.1349-04.2319-04.6039-04.1236-03.1885-03.1326-03.8513-04.5035-04
107.    .3229-04.2114-04.1509-04.1178-04
108.    .1880-09.6446-09.1717-08.3000-08.3328-08.3034-08.2407-08.1853-08.3531-07.1334-06
109.    .3738-06.9750-06.2434-05.5819-05.2402-04.6672-04.1154-03.8699-04.6052-04.3986-04
110.    .2797-04.2011-04.1549-04.1243-04
111.    .3575-09.1073-08.2809-08.5235-08.6660-08.7641-08.8406-08.1600-06.5838-06.1274-05
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112.     .2534-05.5049-05.1019-04.2033-04.6352-04.1412-03.2476-03.2558-03.2338-03.2019-03
113.     .1762-03.1536-03.1374-03.1265-03
114.     .2588-01.2587-01.2589-01.2591-01.2592-01.2593-01.2594-01.2595-01.2597-01.2598-01
115.     .2600-01.2601-01.2601-01.2600-01.2600-01.2597-01.2597-01.2595-01.2594-01.2594-01
116.     .2593-01.2593-01.2593-01.2593-01
117.     .6990-09.1839-08.3679-08.4807-08.4786-08.3820-08.2572-08.1332-08.7816-09.3660-09
118.     .1901-09.4019-09.1455-08.5250-08.3904-07.1415-06.9501-07.9348-08.5035-09.1864-10
119.     .6065-12.1746-13.4491-15.1024-16
120.     .1135-07.2250-07.3519-07.4098-07.4092-07.3798-07.3369-07.3147-07.3568-07.5183-07
121.     .8926-07.1676-06.3245-06.6137-06.1628-05.2150-05.5194-06.3478-07.1637-08.6072-10
122.     .2083-11.6469-13.1782-14.4282-16
```

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                     PREMIXED ONE DIMENSIONAL FLAME CODE SOLUTION (PROF)

                  PROGRAM DOCUMENTED IN THE "PROF CODE USER'S MANUAL",
                    AEROTHERM/ACUREX CORP FINAL REPORT 78-277
                            PHONE 415/964-3200


 CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.952

                          * INTEGRAL PARAMETERS *

 COLUMN                                         COLUMN
   3  NO. SPECIES CONSERVATION EQS.  16            6  PROBLEM TYPE AND ENERGY EQ.       3

   9  NO. OF SPECIES                 16           12  NO. AXIAL GRID PTS.              25

  15  NO. GRID SOLUTION ITERATIONS    8           18  SOLUTION CYCLE CONTROL NO.        3

  21  READ INITIAL MOLE FRACTION      1           24  READ NONINTEGRAL PARAMETERS       1

  27  THERMO DATA & HEAT LOSS MODEL  -3           30  CONSTRAINT SWITCH                 1

  33  READ KINETIC DATA               1           36  CONSTRAINT APPLIED TO VARIABLE    1

  39  CONSTRAINT APPLIED TO GRID PT. 12           42  OUTPUT CONTROL NO.                2

  45  FLAMEHOLDER TEMP ASSIGN SWITCH  1           48  INPUT MASS FLOWRATE SWITCH        1


                          * NONINTEGRAL PARAMETERS *

  APR=DEL/MDOT= .30000-01   BP=DBAR/(DEL*MDOT)= .25000+00    P=   1.000(ATM)   TI=   298.0(K)

      TKAP=    .00200   TFLAME=  298.0(K)


    MASS FLOWRATE=  .30000-01

                          * GRID PARAMETERS *

    A(N)**2 ,N=1, 25

    .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
         .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
              .1000+01  .1000+01  .1000+01  .1000+01  .1000+01

    SIGMA(N),N=1, 25
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                              * FIRST GUESS ALPHAS *

CH4/AIR  SAROFIM  P=1ATM  T=298  PHI=.952

         NORMALIZED  S(N),N=1,25

 .5000-01  .5000-01  .5000-01  .5000-01  .5000-01  .5000-01  .5000-01  .5000-01
 .5000-01  .5000-01  .5000-01  .5000-01  .5000-01  .5000-01  .1000+00  .1000+00
 .2000+00  .5000+00  .5000+00  .1000+01  .1000+01  .2000+01  .2000+01  .4000+01
 .4000+01

         ENTHALPY(CAL/GM),N=1,25

-.6040+02 -.6040+02 -.5940+02 -.5800+02 -.5690+02 -.5550+02 -.5390+02 -.5190+02
-.4970+02 -.4720+02 -.4460+02 -.4190+02 -.3960+02 -.3810+02 -.4000+02 -.4970+02
-.6390+02 -.6350+02 -.6090+02 -.5990+02 -.5910+02 -.5890+02 -.5880+02 -.5870+02

         (ALPHA(I,N),I=1,16,N=1,25)

 .3211-02  .3130-02  .3018-02  .2920-02  .2850-02  .2765-02  .2663-02  .2540-02
 .2391-02  .2213-02  .2000-02  .1749-02  .1459-02  .1139-02  .5332-03  .1403-03
 .8115-05  .3037-06  .1238-07  .5227-09  .2185-10  .8520-12  .2843-13  .7919-15
 .6779-02  .6655-02  .6487-02  .6341-02  .6239-02  .6116-02  .5970-02  .5797-02
 .5590-02  .5345-02  .5053-02  .4709-02  .4305-02  .3840-02  .2837-02  .1871-02
 .1065-02  .7948-03  .6733-03  .5866-03  .5256-03  .4812-03  .4503-03  .4309-03
 .1153-04  .2890-04  .5796-04  .8712-04  .1090-03  .1363-03  .1705-03  .2131-03
 .2661-03  .3322-03  .4140-03  .5151-03  .6389-03  .7894-03  .1141-02  .1560-02
 .2204-02  .2575-02  .2738-02  .2856-02  .2941-02  .3009-02  .3056-02  .3087-02
 .2189-03  .4226-03  .6849-03  .8977-03  .1037-02  .1197-02  .1383-02  .1597-02
 .1843-02  .2126-02  .2449-02  .2815-02  .3225-02  .3675-02  .4585-02  .5341-02
 .5840-02  .6004-02  .6131-02  .6239-02  .6314-02  .6365-02  .6401-02  .6422-02
 .1495-03  .2009-03  .2473-03  .2760-03  .2920-03  .3088-03  .3267-03  .3456-03
 .3656-03  .3868-03  .4091-03  .4324-03  .4558-03  .4780-03  .5083-03  .4855-03
 .3734-03  .2982-03  .2429-03  .1850-03  .1457-03  .1147-03  .9449-04  .8167-04
 .2435-04  .5410-04  .9801-04  .1376-03  .1653-03  .1984-03  .2383-03  .2861-03
 .3435-03  .4122-03  .4944-03  .5922-03  .7075-03  .8410-03  .1123-02  .1304-02
 .1030-02  .6998-03  .5438-03  .4271-03  .3444-03  .2772-03  .2303-03  .1999-03
 .1134-04  .2156-04  .3609-04  .4849-04  .5762-04  .6921-04  .8393-04  .1024-03
 .1251-03  .1528-03  .1857-03  .2229-03  .2609-03  .2919-03  .2890-03  .1606-03
 .1801-04  .9666-06  .4494-07  .1811-08  .6829-10  .2345-11  .7027-13  .1799-14
 .1033-05  .2046-05  .3443-05  .4609-05  .5367-05  .6217-05  .7159-05  .8200-05
 .9371-05  .1072-04  .1230-04  .1406-04  .1572-04  .1659-04  .1329-04  .6032-05
 .4928-06  .1324-07  .3431-09  .9178-11  .1066-11  .5619-12  .3825-12  .2874-12
 .1468-11  .9261-11  .3293-10  .6421-10  .5894-10  .2805-10  .2149-10  .1386-09
 .5622-09  .1731-08  .4844-08  .1327-07  .3565-07  .8995-07  .3512-06  .4929-06
 .9734-07  .5350-08  .1360-08  .7982-09  .5414-09  .3769-09  .2856-09  .2354-09
 .2175-06  .7213-06  .1661-05  .2430-05  .2801-05  .3070-05  .3202-05  .3207-05
 .3136-05  .3064-05  .3065-05  .3187-05  .3411-05  .3608-05  .3064-05  .1462-05
 .2783-06  .1340-06  .9411-07  .6491-07  .4599-07  .3301-07  .2529-07  .2093-07
 .4782-11  .3758-10  .3956-09  .2107-08  .4409-08  .7727-08  .1206-07  .1420-06
 .9069-06  .2184-05  .4276-05  .7723-05  .1349-04  .2319-04  .6039-04  .1236-03
 .1885-03  .1326-03  .8513-04  .5035-04  .3229-04  .2114-04  .1509-04  .1178-04
 .1880-09  .6446-09  .1717-08  .3000-08  .3328-08  .3034-08  .2407-08  .1853-08
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.3531-07  .1334-06  .3738-06  .9750-06  .2434-05  .5819-05  .2402-04  .6672-04
.1154-03  .8659-04  .6052-04  .3986-04  .2797-04  .2011-04  .1549-04  .1283-04
.3575-09  .1073-08  .2809-08  .5295-08  .6660-08  .7641-08  .8406-08  .1600-06
.5838-06  .1274-05  .2534-05  .5049-05  .1019-04  .2033-04  .6352-04  .1412-03
.2476-03  .2558-03  .2338-03  .2019-03  .1762-03  .1536-03  .1374-03  .1265-03
.2588-01  .2587-01  .2589-01  .2591-01  .2592-01  .2593-01  .2594-01  .2595-01
.2597-01  .2598-01  .2600-01  .2601-01  .2601-01  .2600-01  .2600-01  .2597-01
.2597-01  .2595-01  .2594-01  .2594-01  .2593-01  .2593-01  .2593-01  .2593-01
.6990-09  .1839-08  .3679-08  .4807-08  .4786-08  .3820-08  .2572-08  .1332-08
.7816-09  .3660-09  .1901-09  .4019-09  .1455-08  .5250-08  .3904-07  .1415-06
.9501-07  .9348-08  .5035-09  .1864-10  .6065-12  .1746-13  .4491-15  .1024-16
.1135-07  .2250-07  .3519-07  .4098-07  .4092-07  .3798-07  .3369-07  .3147-07
.3568-07  .5183-07  .8926-07  .1676-06  .3245-06  .6137-06  .1628-05  .2150-05
.5194-06  .3478-07  .1637-08  .6072-10  .2083-11  .6469-13  .1782-14  .4282-16

         APHH= .40331-01      BPR= .25000+00


SCALED  H AND ALPHA FIRST GUESS VALUES

    H(N),N=1, 25

 -.58691+02  -.60400+02  -.60400+02  -.59400+02  -.58000+02  -.56900+02  -.55500+02  -.53900+02
     -.51900+02  -.49700+02  -.47200+02  -.44600+02  -.41900+02  -.39600+02  -.38100+02  -.40000+02
         -.49700+02  -.63900+02  -.63500+02  -.60900+02  -.59900+02  -.59100+02  -.58900+02  -.58800+02
             -.58700+02

 ALPHA(I,N),I=1,16,N=1,25

  .32867-02   .32110-02   .31300-02   .30160-02   .29200-02   .28500-02   .27650-02   .26630-02
      .25400-02   .23910-02   .22130-02   .20000-02   .17490-02   .14590-02   .11390-02   .53320-03
          .14030-03   .81150-05   .30370-06   .12380-07   .52270-09   .21850-10   .85200-12   .28430-13
              .79190-15
  .68984-02   .67790-02   .66550-02   .64870-02   .63410-02   .62390-02   .61160-02   .59700-02
      .57970-02   .55900-02   .53450-02   .50530-02   .47090-02   .43050-02   .38400-02   .28370-02
          .18710-02   .10650-02   .79480-03   .67330-03   .58660-03   .52560-03   .48120-03   .45030-03
              .43090-03
  .36118-10   .11520-04   .28900-04   .57960-04   .87120-04   .10900-03   .13630-03   .17050-03
      .21310-03   .26610-03   .33220-03   .41400-03   .51510-03   .63890-03   .78940-03   .11410-02
          .15600-02   .22040-02   .25750-02   .27380-02   .28560-02   .29410-02   .30090-02   .30560-02
              .30870-02
  .36118-10   .21890-03   .42260-03   .68490-03   .89770-03   .10370-02   .11970-02   .13830-02
      .15970-02   .18430-02   .21260-02   .24490-02   .28150-02   .32250-02   .36750-02   .45850-02
          .53410-02   .58400-02   .60040-02   .61310-02   .62390-02   .63140-02   .63650-02   .64010-02
              .64220-02
  .36118-10   .14950-03   .20090-03   .24730-03   .27600-03   .29200-03   .30880-03   .32670-03
      .34560-03   .36560-03   .38680-03   .40910-03   .43240-03   .45580-03   .47800-03   .50830-03
          .48550-03   .37340-03   .29820-03   .24290-03   .18500-03   .14570-03   .11470-03   .94490-04
              .81670-04
  .36118-10   .24350-04   .54100-04   .98010-04   .13760-03   .16530-03   .19840-03   .23830-03
      .28610-03   .34350-03   .41220-03   .49440-03   .59220-03   .70750-03   .84100-03   .11230-02
          .13040-02   .10300-02   .69980-03   .54380-03   .42710-03   .34440-03   .27720-03   .23030-03
              .19990-03
  .36118-10   .11340-04   .21960-04   .36090-04   .48490-04   .57620-04   .69210-04   .83930-04
      .10240-03   .12510-03   .15280-03   .18570-03   .22290-03   .26040-03   .29190-03   .28900-03
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          .16060-03   .18010-04   .96660-06   .44940-07   .18110-08   .68290-10   .23450-11   .70270-13
              .17990-14
.36118-10   .10330-05   .20460-05   .34430-05   .46090-05   .53670-05   .62170-05   .71590-05
     .82000-05   .93710-05   .10720-04   .12300-04   .14060-04   .15720-04   .16590-04   .13290-04
          .60320-05   .49280-06   .13240-07   .34310-09   .91780-11   .10660-11   .56190-12   .38250-12
              .28740-12
.36118-10   .14680-11   .92610-11   .32930-10   .64210-10   .58940-10   .28050-10   .21490-10
     .13860-09   .56220-09   .17310-08   .48440-08   .13270-07   .35650-07   .89950-07   .33120-06
          .49290-06   .97340-07   .53500-08   .13600-08   .79820-09   .54140-09   .37690-09   .28560-09
              .23540-09
.36118-10   .21750-06   .72130-06   .16610-05   .24300-05   .28010-05   .30700-05   .32020-05
     .32070-05   .31360-05   .30640-05   .30650-05   .31870-05   .34110-05   .36080-05   .30640-05
          .14620-05   .27830-06   .13400-06   .94110-07   .64910-07   .45990-07   .33010-07   .25290-07
              .20930-07
.36118-10   .47820-11   .37980-10   .39560-09   .21070-08   .44090-08   .77270-08   .12060-07
     .14200-06   .90690-06   .21840-05   .42760-05   .77230-05   .13490-04   .23190-04   .60390-04
          .12360-03   .18850-03   .13260-03   .85130-04   .50350-04   .32290-04   .21140-04   .15090-04
              .11780-04
.36118-10   .18800-09   .64460-09   .17170-08   .30000-08   .33280-08   .30340-08   .24070-08
     18530-08   .35310-07   .13340-06   .37380-06   .97500-06   .24340-05   .58190-05   .24020-04
          .66720-04   .11540-03   .86990-04   .60520-04   .39860-04   .27970-04   .20110-04   .15490-04
              .12830-04
.36118-10   .35750-09   .10730-08   .28090-08   .52950-08   .66600-08   .76410-08   .84060-08
     .16000-06   .58380-06   .12740-05   .25340-05   .50490-05   .10190-04   .20330-04   .63520-04
          .14120-03   .24760-03   .25580-03   .23980-03   .20190-03   .17620-03   .15360-03   .13740-03
              .12650-03
.25932-01   .25880-01   .25870-01   .25890-01   .25910-01   .25920-01   .25930-01   .25940-01
     .25950-01   .25970-01   .25980-01   .26000-01   .26010-01   .26010-01   .26000-01   .26000-01
          .25970-01   .25970-01   .25950-01   .25940-01   .25940-01   .25930-01   .25930-01   .25930-01
              .25930-01
.36118-10   .69900-09   .18390-08   .36790-08   .48070-08   .47860-08   .38200-08   .25720-08
     .13320-08   .78160-09   .36600-09   .19010-09   .40190-09   .14550-08   .52500-08   .39040-07
          .14150-06   .95010-07   .93480-08   .50350-09   .18640-10   .60650-12   .17460-13   .44910-15
              .10240-16
.36118-10   .11350-07   .22500-07   .35190-07   .40980-07   .40920-07   .37980-07   .33690-07
     .31470-07   .35680-07   .51830-07   .89260-07   .16760-06   .32450-06   .61370-06   .16280-05
          .21500-05   .51940-06   .34780-07   .16370-08   .60720-10   .20830-11   .64690-13   .17820-14
              .42820-16
```

```
                    * GRID INFORMATION SUMMARY TABLE *

ITERATION=   6       NUMBER OF GRID POINTS=  25


 FLAME SPEED PAR= .67391-01          FLAME SPEED= .26495+02 CM/SEC


 GRID COORDINATES(CM)

  .00000      .14494-02   .29338-02   .45069-02   .61778-02   .79570-02   .98560-02   .11886-01
      .14061-01   .16391-01   .18892-01   .21574-01   .24450-01   .27533-01   .30836-01   .38108-01
          .46227-01   .64053-01   .11172+00   .16117+00   .26218+00   .36458+00   .57103+00   .77842+00
              .11939+01

NONDIMENSIONAL GRID INCREMENTS
  .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .50000-01
      .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .50000-01   .10000+00   .10000+00
          .20000+00   .50000+00   .50000+00   .10000+01   .10000+01   .20000+01   .20000+01   .40000+01
              .40000+01

TIME(SEC)

  .00000      .54430-04   .10751-03   .15893-03   .20863-03   .25663-03   .30293-03   .34756-03
      .39054-03   .43188-03   .47163-03   .50983-03   .54653-03   .58180-03   .61574-03   .68015-03
          .74082-03   .85711-03   .11420-02   .14251-02   .19897-02   .25538-02   .36818-02   .48105-02
              .70707-02

ENTHALPY(CAL/GM)

 -.58691+02  -.10161+03  -.10084+03  -.10001+03  -.99023+02  -.97832+02  -.96448+02  -.94869+02
     -.93094+02  -.91158+02  -.89085+02  -.86982+02  -.84958+02  -.83213+02  -.82107+02  -.83322+02
         -.92093+02  -.10802+03  -.10773+03  -.10602+03  -.10613+03  -.10692+03  -.10885+03  -.11156+03
             -.11520+03

TEMPERATURE(K)

  .29800+03   .29800+03   .32506+03   .35610+03   .39162+03   .43218+03   .47840+03   .53095+03
      .59051+03   .65772+03   .73319+03   .81746+03   .91096+03   .10139+04   .11261+04   .13582+04
          .15811+04   .17905+04   .19082+04   .19724+04   .20151+04   .20406+04   .20552+04   .20613+04
              .20604+04

DENSITY(GM/CM3)

  .11323-02   .11209-02   .10272-02   .93673-03   .85080-03   .77028-03   .69525-03   .62587-03
      .56220-03   .50414-03   .45170-03   .40452-03   .36244-03   .32518-03   .29249-03   .24206-03
          .20794-03   .18453-03   .17432-03   .16925-03   .16615-03   .16438-03   .16344-03   .16311-03
              .16329-03

SYSTEM MOLECULAR WEIGHT
```

```
.27687+02   .27409+02   .27401+02   .27372+02   .27340+02   .27317+02   .27293+02   .27269+02
     .27242+02   .27209+02   .27176+02   .27134+02   .27091+02   .27054+02   .27028+02   .26976+02
          .26979+02   .27113+02   .27296+02   .27395+02   .27474+02   .27524+02   .27564+02   .27590+02
               .27608+02
```

```
* MOLE FRACTIONS OF  16  SPECIES *

CH4
.91000-01  .82463-01  .81152-01  .79625-01  .77858-01  .75813-01  .73440-01  .70683-01
   .67477-01  .63740-01  .59375-01  .54267-01  .48308-01  .41421-01  .33644-01  .17590-01
      .51239-02  .25893-03  .87480-05  .34378-06  .14530-07  .63009-09  .26271-10  .98855-12
         .33241-13
O2
.19100+00  .17746+00  .17543+00  .17306+00  .17032+00  .16716+00  .16350+00  .15925+00
   .15432+00  .14860+00  .14198+00  .13431+00  .12546+00  .11528+00  .10366+00  .78017-01
      .51333-01  .26612-01  .19282-01  .16179-01  .14065-01  .12655-01  .11657-01  .10965-01
         .10500-01
CO2
.10000-08  .18216-02  .22214-02  .27083-02  .33013-02  .40236-02  .49031-02  .59735-02
   .72758-02  .88596-02  .10784-01  .13120-01  .15951-01  .19369-01  .23472-01  .33070-01
      .44895-01  .64117-01  .74463-01  .78840-01  .81986-01  .84123-01  .85794-01  .86962-01
         .87776-01
H2O
.10000-08  .19377-01  .21998-01  .24970-01  .28340-01  .32163-01  .36496-01  .41408-01
   .46974-01  .53277-01  .60411-01  .68472-01  .77551-01  .87713-01  .98943-01  .12247+00
      .14422+00  .16072+00  .16680+00  .17081+00  .17393+00  .17597+00  .17739+00  .17837+00
         .17904+00
H2
.10000-08  .57793-02  .60665-02  .63676-02  .66834-02  .70147-02  .73619-02  .77261-02
   .81081-02  .85091-02  .89307-02  .93749-02  .98430-02  .10331-01  .10823-01  .11655-01
      .11515-01  .86487-02  .65575-02  .50811-02  .36701-02  .27635-02  .20609-02  .15979-02
         .12796-02
CO
.10000-08  .22947-02  .27046-02  .31871-02  .37551-02  .44238-02  .52107-02  .61367-02
   .72258-02  .85063-02  .10011-01  .11779-01  .13851-01  .16272-01  .19076-01  .25259-01
      .30274-01  .23442-01  .14924-01  .11072-01  .82324-02  .63055-02  .47760-02  .37096-02
         .29641-02
CH3
.10000-08  .11592-02  .13128-02  .14864-02  .16829-02  .19052-02  .21569-02  .24428-02
   .27710-02  .31550-02  .36142-02  .41704-02  .48373-02  .55972-02  .63554-02  .70728-02
      .47351-02  .50082-03  .24648-04  .10928-05  .43262-07  .16653-08  .60197-10  .19992-11
         .60349-13
CH2O
.10000-08  .70546-04  .80092-04  .90921-04  .10321-03  .11716-03  .13300-03  .15101-03
   .17154-03  .19504-03  .22213-03  .25355-03  .28945-03  .32717-03  .35699-03  .32975-03
      .17752-03  .13958-04  .31584-06  .74197-08  .18109-09  .15294-10  .65161-11  .38766-11
         .24855-11
CHO
.10000-08  .20944-11  .36425-11  .77396-11  .17951-10  .44332-10  .11922-09  .33995-09
   .10685-08  .34052-08  .10597-07  .31828-07  .93628-07  .27327-06  .77628-06  .39514-05
      .91705-05  .23711-05  .10769-06  .23939-07  .12572-07  .76171-08  .45890-08  .29532-08
```

```
                    .20191-08
H02

  .10000-08   .14600-04   .17442-04   .20833-04   .24876-04   .29693-04   .35416-04   .42151-04
        .49828-04   .57893-04   .65232-04   .70821-04   .74752-04   .78262-04   .81829-04   .77821-04
              .44484-04   .76063-05   .33662-05   .22752-05   .15050-05   .10300-05   .70921-06   .51856-06
                    .40393-06
H

  .10000-08   .18298-11   .10911-12   .57375-12   .49190-11   .50647-08   .53092-07   .37269-06
        .18023-05   .63496-05   .17540-04   .40619-04   .83559-04   .16021-03   .29637-03   .87238-03
              .21484-02   .39370-02   .25482-02   .15105-02   .82755-03   .49961-03   .30448-03   .20023-03
                    .14035-03
O

  .10000-08   .10483-08   .16626-08   .32050-08   .64523-08   .13068-07   .26803-07   .55980-07
        .12699-06   .31108-06   .84259-06   .24369-05   .71421-05   .20397-04   .55796-04   .28553-03
              .10270-02   .23194-02   .16506-02   .10801-02   .67242-03   .45275-03   .31010-03   .22574-03
                    .17296-03
HO

  .10000-08   .26090-07   .35803-07   .57238-07   .10146-06   .19490-06   .40448-06   .90296-06
        .21103-05   .49164-05   .11006-04   .23643-04   .50050-04   .10721-03   .23219-03   .87551-03
              .24530-02   .53280-02   .54468-02   .48220-02   .40257-02   .34145-02   .28817-02   .24819-02
                    .21755-02
N2

  .71800+00   .70983+00   .70932+00   .70873+00   .70815+00   .70758+00   .70700+00   .70640+00
        .70578+00   .70515+00   .70454+00   .70397+00   .70348+00   .70311+00   .70282+00   .70230+00
              .70203+00   .70409+00   .70830+00   .71060+00   .71259+00   .71382+00   .71483+00   .71549+00
                    .71595+00
CH

  .10000-08   .29495-10   .32385-10   .36762-10   .44313-10   .59006-10   .59798-10   .20765-08
        .11663-10   .55746-11   .29577-11   .27367-09   .44286-08   .78482-08   .33192-07   .32964-06
              .20075-05   .21198-05   .19453-06   .94703-08   .32217-09   .10118-10   .28848-12   .76972-14
                    .19046-15
CH2

  .10000-08   .51823-07   .58407-07   .66098-07   .75560-07   .88290-07   .10755-06   .14013-06
        .19945-06   .31082-06   .52237-06   .93340-06   .17630-05   .35150-05   .71908-05   .24122-04
              .45932-04   .13146-04   .80942-06   .35318-07   .12471-08   .42556-10   .13517-11   .39997-13
                    .10900-14
```

Another important difference between this sample case and the free flame case is the distribution of grid spacings. For the flameholder problem it is expected that the flame zone or "action zone" will approach the flameholder. To define gradients in this region the grid spacings must be made small. Unlike the free flame case where grid spacings go from relatively large values at the upstream boundary to small values at the constraint, the flameholder calculation uses small grid spacings from the upstream boundary to the constraint. This can be seen in the input listing. Downstream of the constraint, where gradients are less steep, larger grid spacings are applied.

As in the free flame calculation, a constraint condition is applied in this problem. This fixes the value of a variable at the constraint value at a given grid location. The value assigned can be arbitrarily selected within the bounds of the minimum and maximum values found for the variable within the flame. Typically a value midway between the pre- and post-flame value is selected. The grid location where the constraint is applied, should be in the middle of the grid where the zone of maximum action is expected. The constraint is not fixed at a given physical location in space. The constraint applied in this case is used to adjust the physical spacing of the grid rather than to determine flame speed. This adjustment is important since the spatial extent of the flame is unknown prior to the solution. The automatic adjustment of the grid places the points where they are needed to define steep gradients.

The grid spacings on the first guess input are altered to be consistent with the current problem grid spacings. This important change is made in anticipation of the flame moving close to the flameholder. This grid spacing has been found to give better first guesses than the typical free flame grid spacing.

The output from this calculation is similar to sample case 1 output. The summary output information given on the following pages illustrates the main differences between sample case 1 and 2 results. The flame speed difference and temperature difference at the second grid point are obvious. The enthalpy decrease at the second grid point for this case is an indication of the amount of energy loss at the flameholder. A comparison of final temperatures between the two cases also indicates that energy has been lost to the flameholder.

In the flameholder case, the flame lies very close to the flameholder. However, the actual spatial extent of the flame or "action" zone is probably not significantly different from the free flame results presented in sample case 1. For lower mass flowrates and greater flameholder losses, the spatial extent of the flame will be significantly different from the free flame case.

7.3 Sample Case 3 - Methane/Air Chemical Evolution in an Internal Combustion Engine

This sample case demonstrates the PROF time evolution chemical kinetic option. The problem consists of an unburnt mixture of methane and air which is subjected to an assigned pressure and temperature history. This problem represents the chemical reaction history of the last element of fuel and air to be burned during the expansion stroke of an internal combustion engine. Initial concentration of methane is 5.9 percent and the initial temperature and pressure are 2393°K and 54.2 atmosphere respectively. The calculation is carried out over four decades in time.

Most of the input for this problem is straightforward. The APR and AP(N) parameters are input in the form suggested in the input guide. For this sample case, APR is set equal to 1 and AP(2) is set equal to the time step between the initial and second station, etc. Since APR and AP(N) are multiplicative, the time step can be distributed between these in any manner as long as the product equals the required value. Input unique to this type

SAMPLE PROBLEM 7.3

```
  1.      TIME EVOLUTION PROBLEM
  2.     14  1 14 30  1  0  1  1 -1  0  1  0  0  2  0  0
  3.         1.      0.      54.2      2393.               2393.
  4.     1.0  E-09 2.0  E-09 7.0  E-09 2.0  F-08 3.0  E-08 4.0  E-08 2.0  E-07 3.0  E-07
  5.     4.0  E-07 2.0  E-06 2.0  E-06 2.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06
  6.     1.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06 1.0  E-06
  7.     1.0  E-06 5.0  E-06 5.0  E-06 1.0  E-05 1.0  E-05 2.0  E-05 3.0  E-05 1.0  E-04
  8.    1.        1.        1.        1.        1.        1.        1.        1.
  9.    1.        1.        1.        1.        1.        1.        1.        1.
 10.    1.        1.        1.        1.        1.        1.        1.        1.
 11.    1.        1.        1.        1.        1.        1.        1.        1.
 12.     2393.00   2393.00   2393.00   2393.00   2392.99   2392.99   2392.98   2392.94
 13.     2392.88   2392.81   2392.42   2392.03   2391.64   2391.44   2391.25   2391.05
 14.     2390.86   2390.66   2390.47   2390.27   2390.08   2389.89   2389.69   2389.50
 15.     2389.30   2389.11   2388.14   2387.16   2385.22   2383.28   2379.40   2373.60
 16.     54.20     54.20     54.20     54.20     54.20     54.20     54.20     54.19
 17.     54.19     54.18     54.13     54.08     54.03     54.01     53.98     53.96
 18.     53.94     53.91     53.89     53.86     53.84     53.82     53.79     53.77
 19.     53.74     53.72     53.60     53.48     53.25     53.01     52.54     51.85
 20.    CH4        .05985         1.-31.0523
 21.    O2         .19751         1.-31.0468
 22.    CO2             1.-9      1.-3 .8
 23.    H2O             1.-9      1.-31.2980
 24.    H2              1.-9      .1-3  3.5333
 25.    CO              1.-9      .1-3  .9830
 26.    CH3             1.-9      .1-3   1.3257
 27.    CH2O            1.-9      .1-3 1.298
 28.    CHO             1.-9      .1-3 .9604
 29.    HO2             1.-9      .1-3  .9016
 30.    H               1.-9      .1-3 5.1557
 31.    O               1.-9      .1-3  1.4158
 32.    HO              1.-9      .1-3  1.3475
 33.    N2         .74264    .74264    .9732
 34.    END
 35.     23
 36.    CO   O2        CO2  O            1.00+13       0.0     60.
 37.    H2O        M   HO   H            3.00+15       0.0       105.0
 38.    H2         M   H    H            2.00+14    0.0     96.
 39.    O2         M   O    O            2.50+19  -1.     118.7
 40.    CH4  HO        CH3  H2O          3.00+13    0.0    5.000
 41.    HO   HO        H2O  O            6.00+12    0.0    1.00
 42.    HO   O         H    O2           2.50+13    0.0    0.00
 43.    H    HO        H2   O            8.00+09     1.    7.00
 44.    H    HO2       HO   HO           2.50+14           1.9
 45.    CH4  O         CH3  HO           1.00+10     1.    8.00
 46.    CH4  H         CH3  H2           5.00+10     1.    10.0
 47.    CH4        M   CH3  H            2.00+17     0.     88.
 48.    CH3  O         CH2O H            2.00+12     .5    -.30
 49.    CH3  O2        CH2O HO           3.00+13    0.0     30.
 50.    CH2O HO        CHO  H2O          3.00+09    1.0    1.0
 51.    CH2O H         CHO  H2           1.25+10    1.0    3.2
 52.    CH2O O         CHO  HC           2.00+11     1.    4.40
 53.    CHO  O         CO   HO           3.00+11     1.    0.50
 54.    CO2        M   CO   O            1.00+15    0.0    100.
```

```
                                                    4.00+09    .5        .0
55.    CO   HO          CO2  H                      1.50+15   0.0      1.00
56.    H    O2     M    HO2                         2.50+15   0.0      5.20
57.    HO   H2          H    H2O                    3.00+10    1.      0.00
58.    CHO  HO          CO   H2O
```

```
                    PREMIXED ONE DIMENSIONAL FLAME CODE SOLUTION (PROF)

                 PROGRAM DOCUMENTED IN THE "PROF CODE USER'S MANUAL",
                   AEROTHERM/ACUREX CORP FINAL REPORT 78-277
                           PHONE 415/964-3200


   TIME EVOLUTION PROBLEM

                           * INTEGRAL PARAMETERS *

COLUMN                                         COLUMN
   3  NO. SPECIES CONSERVATION EQS.  14            6  PROBLEM TYPE AND ENERGY EQ.      1

   9  NO. OF SPECIES                 14           12  NO. AXIAL GRID PTS.             30

  15  NO. GRID SOLUTION ITERATIONS    1           18  SOLUTION CYCLE CONTROL NO.       0

  21  READ INITIAL MOLE FRACTION      1           24  READ NONINTEGRAL PARAMETERS      1

  27  THERMO DATA & HEAT LOSS MODEL  -1           30  CONSTRAINT SWITCH                0

  33  READ KINETIC DATA               1           36  CONSTRAINT APPLIED TO VARIABLE  0

  39  CONSTRAINT APPLIED TO GRID PT.  0           42  OUTPUT CONTROL NO.               2

  45  FLAMEHOLDER TEMP ASSIGN SWITCH  0           48  INPUT MASS FLOWRATE SWITCH       0


                           * NONINTEGRAL PARAMETERS *

   APR=DEL/MDOT= .10000+01   BP=DBAR/(DEL*MDOT)= .00000       P=  54.200(ATM)   TI=  2393.0(K)

        TKAP=    .00000   TFLAME= 2393.0(K)


                             * GRID PARAMETERS *

      A(N)**2 ,N=1, 30

       .1000-08  .2000-08  .7000-08  .2000-07  .3000-07  .4000-07  .2000-06  .3000-06  .4000-06  .2000-05
            .2000-05  .2000-05  .1000-05  .1000-05  .1000-05  .1000-05  .1000-05  .1000-05  .1000-05  .1000-05
                 .1000-05  .1000-05  .1000-05  .1000-05  .1000-05  .5000-05  .5000-05  .1000-04  .1000-04  .2000-04

      SIGMA(N),N=1, 30

       .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
            .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
                 .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
                 * ASSIGNED T AND P DISTRIBUTION *

TEMPERATURE DISTRIBUTION (K)
   .23930+C4   .23930+04   .23930+04   .23930+04   .23930+04   .23930+04   .23930+04   .23929+04
       .23929+04   .23928+04   .23924+04   .23920+04   .23916+04   .23914+04   .23912+04   .23910+04
           .23909+04   .23907+04   .23905+04   .23903+04   .23901+04   .23899+04   .23897+04   .23895+04
               .23893+04   .23891+04   .23881+04   .23872+04   .23852+04   .23833+04

PRESSURE CISTRIBUTION(ATM)
   .54200+C2   .54200+02   .54200+02   .54200+02   .54200+02   .54200+02   .54200+02   .54190+02
       .54190+02   .54180+02   .54130+02   .54080+02   .54030+02   .54010+02   .53980+02   .53960+02
           .53940+02   .53910+02   .53890+02   .53860+02   .53840+02   .53820+02   .53790+02   .53770+02
               .53740+02   .53720+02   .53600+02   .53480+02   .53250+02   .53010+02
```

```
* SPECIES INITIAL MOLE FRACTIONS.FIRST GUESSES.AND DIFFUSION FACTORS *

SPECIE                   ALPF              ALPE          DIFFUSION FACTOR

 CH4                    .598-01           .100-02             1.0523
 O2                     .198+00           .100-02             1.0468
 CO2                    .100-08           .100-02              .8000
 H2O                    .100-08           .100-02             1.2980
 H2                     .100-08           .100-03             3,5333
 CO                     .100-08           .100-03              .9830
 CH3                    .100-08           .100-03             1.3257
 CH2O                   .100-08           .100-03             1.2980
 CHO                    .100-08           .100-03              .9604
 HO2                    .100-08           .100-03              .9016
 H                      .100-08           .100-03             5,1557
 O                      .100-08           .100-03             1.4158
 HO                     .100-08           .100-03             1.3475
 N2                     .743+00           .743+00              .9732
```

* THERMOCHEMISTRY DATA *

```
        CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/FOL)  H(CAL/MOL)      RB           RC           RD        S(CAL/MOL/K)      TU(K)      NAME

   CO           28.011
-.26417+05   .25539+05   .58640+01   .21499-02    .42295+05    .66789+02   300.  1000.   CO
-.26417+05   .22179+05   .57638+01   .11821-02    .11103+07    .65218+02  1000.  2500.   CO
   CO2          44.011
-.94054+05   .41438+05   .95778+01   .36020-02   -.16389+06    .81997+02   300.  1000.   CO2
-.94054+05   .36573+05   .13972+02   .38449-03   -.13412+07    .79867+02  1000.  2500.   CO2
   CH4          16.043
-.17895+05   .66727+05   .56930+01   .11565-01   -.66950+05    .88496+02   300.  1000.   CH4
-.17895+05   .53270+05   .20336+02   .16707-02   -.48155+07    .82684+02  1000.  2500.   CH4
   H2O          18.016
-.57798+05   .31716+05   .68290+01   .29575-02    .27843+05    .69022+02   300.  1000.   H2O
-.57798+05   .30303+05   .99698+01   .12774-02   -.14328+07    .68463+02  1000.  2500.   H2O
   O2           32.000
 .00000      .25541+05   .67044+01   .16795-02   -.19419+05    .68908+02   300.  1000.   O2
 .00000      .23450+05   .80725+01   .50513-03   -.21319+06    .67976+02  1000.  2500.   O2
   N2           28.016
 .79000+00   .23993+05   .61391+01   .16415-02    .29727+05    .64548+02   300.  1000.   N2
 .79000+00   .22188+05   .83049+01   .23357-03   -.72806+06    .63774+02  1000.  2500.   N2
   H2            2.016
 .20000+00   .20180+05   .67559+01   .43063-03    .21903+04    .47986+02   300.  1000.   H2
 .20000+00   .21258+05   .65812+01   .82395-03   -.21635+06    .48484+02  1000.  2500.   H2
   H             1.008
 .52100+05   .13423+05   .49680+01  -.79563-08   -.65188+00    .38862+02   300.  1000.   H
 .52100+05   .13423+05   .49680+01  -.21457-08   -.38277+01    .38862+02  1000.  2500.   H
   O            16.000
 .59559+05   .13449+05   .50132+01  -.35760-04    .21105+05    .50064+02   300.  1000.   O
 .59559+05   .13517+05   .49475+01   .10904-04    .40118+05    .50094+02  1000.  2500.   O
   HO           17.008
 .94320+04   .21099+05   .64878+01   .77321-03    .41428+05    .61183+02   300.  1000.   HO
 .94320+04   .21452+05   .72179+01   .58712-03   -.50251+06    .61372+02  1000.  2500.   HO
   HO2          33.008
 .50000+04   .36387+05   .82485+01   .32199-02   -.82934+05    .81654+02   300.  1000.   HO2
 .50000+04   .32593+05   .12102+02   .54010-03   -.12571+07    .80006+02  1000.  2500.   HO2
   CH3          15.035
 .34820+05   .48677+05   .80457+01   .60835-02   -.58069+05    .81068+02   300.  1000.   CH3
 .34820+05   .42779+05   .15742+02   .12359-02   -.29064+07    .78562+02  1000.  2500.   CH3
   CH2O         30.027
-.27700+05   .54354+05   .68621+01   .80908-02   -.82595+05    .89490+02   300.  1000.   CH2O
-.27700+05   .43898+05   .17110+02   .85504-03   -.30943+07    .84938+02  1000.  2500.   CH2O
   CHO          29.019
-.29000+04   .37003+05   .74602+01   .38023-02   -.33115+05    .80992+02   300.  1000.   CHO
-.29000+04   .32424+05   .12304+02   .49109-03   -.15653+07    .79009+02  1000.  2500.   CHO
```

```
                    * KINETIC REACTION DATA *

      NUMBER OF REACTIONS= 23

 M              REACTION                              PRE EXP FACTOR  TEMP EXP      ACTIVATION      INDIVIDUAL THIRD BODY EFFIC.
                                                       (MOLE-CM-S)                  (KCAL/MOLE)     NAME1      ETB1   NAME2      ETB2

 1   CO   +O2   +      --=   CO2  +O                  .1000+14+ 0.     .000          60.0000                   .000             .000
 2   H2O  +     +M     --=   HO   +H                  .3000+16+ 0.     .000         105.0000                   .000             .000
 3   H2   +     +M     --=   H    +H                  .2000+15+ 0.     .000          96.0000                   .000             .000
 4   O2   +     +M     --=   O    +O                  .2500+20+ 0.   -1.000         118.7000                   .000             .000
 5   CH4  +HO   +      --=   CH3  +H2O                .3000+14+ 0.     .000           5.0000                   .000             .000
 6   HO   +HO   +      --=   H2O  +O                  .6000+13+ 0.     .000           1.0000                   .000             .000
 7   HO   +O    +      --=   H    +O2                 .2500+14+ 0.     .000            .0000                   .000             .000
 8   H    +HO   +      --=   H2   +O                  .8000+10+ 0.    1.000           7.0000                   .000             .000
 9   H    +HO2  +      --=   HO   +HO                 .2500+15+ 0.     .000           1.9000                   .000             .000
10   CH4  +O    +      --=   CH3  +HO                 .1000+11+ 0.    1.000           8.0000                   .000             .000
11   CH4  +H    +      --=   CH3  +H2                 .5000+11+ 0.    1.000          10.0000                   .000             .000
12   CH4  +     +M     --=   CH3  +H                  .2000+18+ 0.     .000          88.0000                   .000             .000
13   CH3  +O    +      --=   CH2O+H                   .2000+13+ 0.     .500           -.3000                   .000             .000
14   CH3  +O2   +      --=   CH2O+HO                  .3000+14+ 0.     .000          30.0000                   .000             .000
15   CH2O+HO    +      --=   CHO  +H2O                .3000+10+ 0.    1.000           1.0000                   .000             .000
16   CH2O+H     +      --=   CHO  +H2                 .1250+11+ 0.    1.000           3.2000                   .000             .000
17   CH2O+O     +      --=   CHO  +HO                 .2000+12+ 0.    1.000           4.4000                   .000             .000
18   CHO  +O    +      --=   CO   +HO                 .3000+12+ 0.    1.000            .5000                   .000             .000
19   CO2  +     +M     --=   CO   +O                  .1000+16+ 0.     .000         100.0000                   .000             .000
20   CO   +HO   +      --=   CO2  +H                  .4000+10+ 0.     .500            .0000                   .000             .000
21   H    +O2   +M     --=   HO2  +                   .1500+16+ 0.     .000           1.0000                   .000             .000
22   HO   +H2   +      --=   H    +H2O                .2500+14+ 0.     .000           5.2000                   .000             .000
23   CHO  +HO   +      --=   CO   +H2O                .3000+11+ 0.    1.000            .0000                   .000             .000
```

```
                    * GRID INFORMATION SUMMARY TABLE *

ITERATION=   1        NUMBER OF GRID POINTS=  30


 GRID COORDINATES(CM)

  .00000     .00000     .00000     .00000     .00000     .00000     .00000     .00000
      .00000     .00000     .00000     .00000     .00000     .00000     .00000     .00000
          .00000     .00000     .00000     .00000     .00000     .00000     .00000     .00000
              .00000     .00000     .00000     .00000     .00000     .00000
NONDIMENSIONAL GRID INCREMENTS
  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01
      .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01
          .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01
              .10000+01  .10000+01  .10000+01  .10000+01  .10000+01  .10000+01
TIME(SEC)

  .00000     .20000-08  .90000-08  .29000-07  .59000-07  .99000-07  .29900-06  .59900-06
      .99900-06  .29990-05  .49990-05  .69990-05  .79990-05  .89990-05  .99990-05  .10999-04
          .11999-04  .12999-04  .13999-04  .14999-04  .15999-04  .16999-04  .17999-04  .18999-04
              .19999-04  .24999-04  .29999-04  .39999-04  .49999-04  .69999-04
ENTHALPY(CAL/GM)

  .61380+03  .61404+03  .61480+03  .61604+03  .61639+03  .61537+03  .59454+03  .55512+03
      .51045+03  .42061+03  .37683+03  .35001+03  .33759+03  .30380+03  .27851+03  .25915+03
          .24566+03  .23636+03  .22984+03  .22513+03  .22165+03  .21900+03  .21693+03  .21530+03
              .21397+03  .21087+03  .20888+03  .20713+03  .20578+03  .20464+03
TEMPERATURE(K)

  .23930+04  .23930+04  .23930+04  .23930+04  .23930+04  .23930+04  .23930+04  .23929+04
      .23929+04  .23928+04  .23924+04  .23920+04  .23916+04  .23914+04  .23912+04  .23910+04
          .23909+04  .23907+04  .23905+04  .23903+04  .23901+04  .23899+04  .23897+04  .23895+04
              .23893+04  .23891+04  .23881+04  .23872+04  .23852+04  .23833+04
DENSITY(GM/CM3)

  .77524-02  .77519-02  .77503-02  .77460-02  .77400-02  .77327-02  .77083-02  .76834-02
      .76613-02  .76043-02  .75696-02  .75501-02  .75407-02  .75660-02  .76014-02  .76302-02
          .76496-02  .76609-02  .76692-02  .76730-02  .76763-02  .76783-02  .76779-02  .76781-02
              .76765-02  .76791-02  .76677-02  .76559-02  .76303-02  .76028-02
SYSTEM MOLECULAR WEIGHT

  .28086+02  .28085+02  .28079+02  .28063+02  .28041+02  .28015+02  .27926+02  .27841+02
      .27760+02  .27558+02  .27453+02  .27403+02  .27390+02  .27490+02  .27631+02  .27744+02
          .27823+02  .27877+02  .27915+02  .27942+02  .27963+02  .27978+02  .27990+02  .27999+02
              .28006+02  .28024+02  .28034+02  .28042+02  .28046+02  .28048+02
```

```
                      * MOLE FRACTIONS OF  14  SPECIES *


 CH4

  .59850-01   .59764-01   .59307-01   .57476-01   .54464-01   .50548-01   .36221-01   .24179-01
        .16609-01   .77028-02   .39123-02   .18724-02   .10424-02   .59794-04   .26103-05   .11396-06
              .53166-08   .26948-09   .14854-10   .88715-12   .57100-13   .39397-14   .29092-15   .23778-16
                    .29513-17   .90703-18   .73212-18   .61687-18   .55102-18   .50506-18

 O2

  .19751+00   .19747+00   .19727+00   .19650+00   .19508+00   .19294+00   .18120+00   .16629+00
        .15231+00   .12705+00   .11514+00   .10807+00   .10483+00   .93509-01   .87039-01   .83356-01
              .81185-01   .79855-01   .79009-01   .78453-01   .78078-01   .77819-01   .77636-01   .77505-01
                    .77411-01   .77237-01   .77173-01   .77147-01   .77147-01   .77153-01

 CO2

  .10000-08   .99995-09   .10105-08   .11225-07   .11547-06   .51870-06   .19786-04   .10442-03
        .28634-03   .16697-02   .31927-02   .51393-02   .66295-02   .20933-01   .33529-01   .41790-01
              .47018-01   .50395-01   .52646-01   .54197-01   .55296-01   .56098-01   .56695-01   .57149-01
                    .57501-01   .58283-01   .58674-01   .58975-01   .59107-01   .59192-01

 H2O

  .10000-08   .77898-05   .13394-03   .93634-03   .25926-02   .51100-02   .18795-01   .36172-01
        .52682-01   .84101-01   .99291-01   .10800+00   .11158+00   .11323+00   .11282+00   .11328+00
              .11393+00   .11452+00   .11501+00   .11541+00   .11574+00   .11600+00   .11623+00   .11641+00
                    .11657+00   .11700+00   .11727+00   .11752+00   .11765+00   .11775+00

 H2

  .10000-08   .10749-04   .69037-04   .27385-03   .59031-03   .94459-03   .14556-02   .14315-02
        .12944-02   .10838-02   .85947-03   .59379-03   .43795-03   .69459-03   .10274-02   .10502-02
              .96117-03   .85395-03   .75620-03   .67347-03   .60486-03   .54812-03   .50103-03   .46165-03
                    .42851-03   .34005-03   .28833-03   .24127-03   .21775-03   .20067-03

 CO

  .10000-08   .10232-08   .10608-06   .19937-04   .12172-03   .34773-03   .29762-02   .84996-02
        .15711-01   .33901-01   .42925-01   .47309-01   .48495-01   .37490-01   .25345-01   .17330-01
              .12270-01   .90092-02   .68390-02   .53469-02   .42899-02   .35212-02   .29491-02   .25144-02
                    .21782-02   .14342-02   .10638-02   .78041-03   .65659-03   .57762-03

 CH3

  .10000-08   .81513-04   .50602-03   .20010-02   .41608-02   .66604-02   .12344-01   .13061-01
        .10235-01   .36810-02   .15512-02   .76004-03   .52560-03   .43961-04   .18713-05   .81797-07
              .39840-08   .21510-09   .12692-10   .80956-12   .55342-13   .40332-14   .31675-15   .30820-16
                    .71790-17   .37734-17   .29650-17   .23422-17   .20116-17   .17862-17

 CH2O

  .10000-08   .59134-06   .20798-04   .27395-03   .88808-03   .18809-02   .70668-02   .12097-01
        .14676-01   .10532-01   .61611-02   .29340-02   .14710-02   .42519-04   .13087-05   .52173-07
              .24921-08   .14592-09   .19050-10   .10410-10   .89421-11   .81059-11   .74448-11   .69002-11
                    .64446-11   .53693-11   .46637-11   .40548-11   .37068-11   .34684-11

 CHO

  .10000-08   .25546-08   .73145-06   .29854-04   .11887-03   .26012-03   .88138-03   .13852-02
        .16368-02   .12368-02   .75759-03   .37873-03   .20252-03   .99952-05   .36467-06   .41628-07
              .22356-07   .17165-07   .13920-07   .11581-07   .98328-08   .84932-08   .74468-08   .66173-08
```

```
          .59498-08   .44058-08   .35291-08   .28132-08   .24572-08   .22205-08
HO2

 .10000-08   .77542-06   .44014-05   .13408-04   .22402-04   .27743-04   .25124-04   .18164-04
     .12442-04   .60058-05   .36033-05   .26079-05   .28257-05   .49070-04   .71223-04   .68952-04
         .61367-04   .53454-04   .46441-04   .40523-04   .35622-04   .31577-04   .28231-04   .25456-04
             .23138-04   .17083-04   .13706-04   .10762-04   .93794-05   .84078-05
H

 .10000-08   .22323-04   .34964-04   .45272-04   .51481-04   .51126-04   .40561-04   .30501-04
     .22587-04   .13158-04   .86997-05   .67088-05   .75599-05   .19870-03   .37617-03   .37729-03
         .32349-03   .26739-03   .22095-03   .18468-03   .15660-03   .13473-03   .11753-03   .10382-03
             .92758-04   .65463-04   .51116-04   .39156-04   .33615-04   .29778-04
O

 .10000-08   .23006-04   .10342-03   .15978-03   .12234-03   .76836-04   .24462-04   .12266-04
     .77870-05   .57213-05   .58359-05   .82909-05   .15909-04   .11178-02   .18163-02   .17937-02
         .15973-02   .13936-02   .12193-02   .10771-02   .96195-03   .86825-03   .79139-03   .72768-03
             .67440-03   .53352-03   .45185-03   .37790-03   .34099-03   .31420-03
HO

 .10000-08   .22528-04   .10492-03   .23923-03   .34115-03   .40742-03   .53837-03   .57212-03
     .50208-03   .35077-03   .30452-03   .35545-03   .53554-03   .57613-02   .73572-02   .73658-02
         .69849-02   .65470-02   .61397-02   .57818-02   .54723-02   .52051-02   .49740-02   .47732-02
             .45979-02   .40966-02   .37718-02   .34504-02   .32746-02   .31399-02
N2

 .74264+00   .74260+00   .74244+00   .74203+00   .74145+00   .74075+00   .73841+00   .73615+00
     .73401+00   .72866+00   .72589+00   .72457+00   .72423+00   .72687+00   .73061+00   .73358+00
         .73567+00   .73711+00   .73811+00   .73884+00   .73937+00   .73977+00   .74008+00   .74033+00
             .74052+00   .74099+00   .74124+00   .74146+00   .74156+00   .74164+00
```

of problem are the temperature and pressure distributions. These values are given for each grid point and are associated with the sum of time steps (i.e. APR*AP(N)) or total time, to that grid point.

The output for this problem is standard except for the printing of temperature and pressure time histories. These appear on the first page of output.

7.4 Sample Case 4 - Methane/Air Well-Stirred Reactor

This sample case demonstrates the PROF code well-stirred reactor option. This problem models a well-stirred combustor operating at 3.4 atmospheres. Initial conditions are 3 percent concentration methane in air at a temperature of 700°K. Five sequential calculations are made for increasing mass rates through the fixed volume reactor. Initial conditons remain the same for these calculations. The increasing mass rates take the calculations in the direction from equilibrium to more kinetically controlled conditions. Typically, the code has the greatest difficulty with solutions near blow-out (i.e., kinetically dominated). Therefore, proceeding from easily obtained near equilibrium solutions to more kinetically controlled solutions increases the probability for solution convergence. To further increase the probability for solution convergence, good estimates for final species concentrations and temperature should be input into the initial species concentration guesses and TFLAME input respectively.

Most of the output is standard for this case. The first station output represents the initial conditions and the following station outputs represent the outlet conditions for the sequence of calculations. In the time output the reactor residence times are printed. These are defined as the reactor volume density product divided by the mass rates through the reactor.

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SAMPLE PROBLEM 7.4

```
 1.     WELL STIRRED REACTOR
 2.    14 -1 14  6  1  0  1  1 -1  0  1  0  0  2  0  0
 3.   .997      0.          3.4         700.         0.         1400.
 4.   1.        100.        50.         25.          12.        6.
 5.   1.        1.          1.          1.           1.         1.
 6.   CH4       .0305            .1-4 1.0525
 7.   O2        .2037       .136      1.04679
 8.   CO2            1.-9 .0200          .8
 9.   H2O            1.-9 .094            1.290
10.   H2             1.-9      .32-4  3.3333
11.   CO             1.-9      .29-3  .9030
12.   CH3            1.-9      .17-4   1.3297
13.   CH2O           1.-9      .29-6 1.290
14.   CHO            1.-9      .29-9 .9604
15.   HO2            1.-9      .29-3  .9016
16.   H              1.-9      .10-5 5.1967
17.   O              1.-9      .23-4  1.4150
18.   HO             1.-9      .15-3  1.3075
19.   N2          .7650     .7650     .9732
20.   END
21.    29
22.   CH4       M   CH3  H              1.50+16   0.0    100.
23.   CH4  HO       CH3  H2O            1.00+13   0.0      6.000
24.   CH4  H        CH3  H2             2.00+14   0.0     11.900
25.   CH4  O        CH3  HO             2.00+14   0.0      6.900
26.   CH3  O        CH2O H              3.50+13   0.0      3.300
27.   CH3  O2       CH2O HO             1.00+12   0.0     15.000
28.   CH2O      M   CO   H2             2.00+16   0.0     35.000
29.   CH2O HO       CHO  H2O            2.50+13   0.0      1.000
30.   CH2O O        CHO  HO             3.00+13   0.0     0.
31.   CH2O H        CHO  H2             1.70+13   0.0      3.000
32.   CHO  O2       CO   HO2            3.00+13   0.0     0.
33.   CHO  HO       CO   H2O            1.00+14   0.0     0.
34.   CHO  O        CO   HO             5.40+11   0.5     0.
35.   CHO       M   CO   H              2.00+12   0.5     20.000
36.   CO   HO       CO2  H              5.50+11   0.0      1.000
37.   CO   O    M   CO2                 3.60+16  -1.0      2.500
38.   HO2  O        O2   HO             2.50+13   0.0     0.
39.   HO2  HO       O2   H2O            2.50+13   0.0     0.
40.   HO2  H        HO   HO             2.50+14   0.0      2.000
41.   HO2  H        O2   H2             2.50+13   0.0       .000
42.   H    O2   M   HO2                 2.00+15   0.0       .870   H2O  20.
43.   H    O2       HO   O              2.20+14   0.0     16.800
44.   O    H2       HO   H              1.70+13   0.0      9.460
45.   HO   H2       H2O  H              2.20+13   0.0      5.200
46.   HO   HO       H2O  O              6.00+12   0.0       .780
47.   H    HO   M   H2O                 7.00+19  -1.0     0.
48.   O    H    M   HO                  4.00+18  -1.0     0.
49.   H    H    M   H2                  2.00+19  -1.0     0.
50.   O    O    M   O2                  4.00+18  -1.0     0.

END ELT.  TIME: 0.3760 SECONDS.
```

```
                    PREMIXED ONE DIMENSIONAL FLAME CODE SOLUTION (PROF)

                  PROGRAM DOCUMENTED IN THE "PROF CODE USER'S MANUAL",
                    AEROTHERM/ACUREX CORP FINAL REPORT 78-277
                               PHONE 415/964-3200


   WELL STIRRED REACTOR


                             * INTEGRAL PARAMETERS *

COLUMN                                         COLUMN
   3  NO. SPECIES CONSERVATION EQS.  14            6  PROBLEM TYPE AND ENERGY EQ.    -1

   9  NO. OF SPECIES                 14           12  NO. AXIAL GRID PTS.             6

  15  NO. GRID SOLUTION ITERATIONS    1           18  SOLUTION CYCLE CONTROL NO.      0

  21  READ INITIAL MOLE FRACTION      1           24  READ NONINTEGRAL PARAMETERS     1

  27  THERMO DATA & HEAT LOSS MODEL  -1           30  CONSTRAINT SWITCH               0

  33  READ KINETIC DATA               1           36  CONSTRAINT APPLIED TO VARIABLE  0

  39  CONSTRAINT APPLIED TO GRID PT.  0           42  OUTPUT CONTROL NO.              2

  45  FLAMEHOLDER TEMP ASSIGN SWITCH  0           48  INPUT MASS FLOWRATE SWITCH      0


                            * NONINTEGRAL PARAMETERS *

   APR=DEL/MCOT= .55700+00   BP=DBAR/(DEL*MDOT)= .00000       P=   3.400(ATM)   TI=   700.0(K)

      TKAF=    .00000   TFLAME= 1400.0(K)


                              * GRID PARAMETERS *

      A(N)**2 ,N=1, 6

      .1000+01  .1000+03  .5000+02  .2500+02  .1200+02  .6000+01

      SIGMA(N),N=1, 6

      .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
```

```
* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSFS,AND DIFFUSION FACTORS *

SPECIE              ALPF           ALPE        DIFFUSION FACTOR

 CH4              .305-01        .100-04          1.0523
 O2               .204+00        .136+00          1.0468
 CO2              .100-08        .288-01           .8000
 H2O              .100-08        .580-01          1.2980
 H2               .100-08        .320-04          3.5333
 CO               .100-08        .240-03           .9830
 CH3              .100-08        .170-04          1.3257
 CH2O             .100-08        .240-06          1.2980
 CHO              .100-08        .240-09           .9604
 HO2              .100-08        .290-05           .9016
 H                .100-08        .100-05          5.1557
 O                .100-08        .230-04          1.4158
 HO               .100-08        .150-U3          1.3475
 N2               .766+00        .766+00           .9732
```

```
                    * THERMOCHEMISTRY DATA *

          CURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (CAL/(MOLE*K)

HF(CAL/MOL)  H(CAL/MOL)     RB           RC           RD        S(CAL/MOL/K)     TU(K)      NAME

    CO          28.011
-.26417+05   .25539+05   .58640+01   .21499-02    .42295+05   .66789+02   300.  1000.    CO
-.26417+05   .22179+05   .57638+01   .11821-02    .11103+07   .65218+02  1000.  2500.    CO
    CO2         44.011
-.94054+05   .41438+05   .95778+01   .36020-02   -.16389+06   .81997+02   300.  1000.    CO2
-.94054+05   .36573+05   .13972+02   .38449-03   -.13412+07   .79867+02  1000.  2500.    CO2
    CH4         16.043
-.17895+05   .66727+05   .56930+01   .11565-01   -.66950+05   .88496+02   300.  1000.    CH4
-.17895+05   .53270+05   .20336+02   .16707-02   -.48155+07   .82684+02  1000.  2500.    CH4
    H2O         18.016
-.57798+05   .31716+05   .68290+01   .29575-02    .27843+05   .69022+02   300.  1000.    H2O
-.57798+05   .30303+05   .99698+01   .12774-02   -.14328+07   .68463+02  1000.  2500.    H2O
    O2          32.000
 .00000      .25541+05   .67044+01   .16795-02   -.19419+05   .68908+02   300.  1000.    O2
 .00000      .23450+05   .80725+01   .50513-03   -.21319+06   .67976+02  1000.  2500.    O2
    N2          28.016
 .79000+00   .23993+05   .61391+01   .16415-02    .29727+05   .64548+02   300.  1000.    N2
 .79000+00   .22188+05   .83049+01   .23357-03   -.72806+06   .63774+02  1000.  2500.    N2
    H2           2.016
 .20000+00   .20180+05   .67559+01   .43063-03    .21903+04   .47986+02   300.  1000.    H2
 .20000+00   .21258+05   .65812+01   .82395-03   -.21635+06   .48484+02  1000.  2500.    H2
    H            1.008
 .52100+05   .13423+05   .49680+01  -.79563-08   -.65188+00   .38862+02   300.  1000.    H
 .52100+05   .13423+05   .49680+01  -.21457-08   -.38277+01   .38862+02  1000.  2500.    H
    O           16.000
 .59559+05   .13449+05   .50132+01  -.35760-04    .21105+05   .50064+02   300.  1000.    O
 .59559+05   .13517+05   .49475+01   .10904-04    .40118+05   .50094+02  1000.  2500.    O
    HO          17.008
 .94320+04   .21099+05   .64878+01   .77321-03    .41428+05   .61183+02   300.  1000.    HO
 .94320+04   .21452+05   .72179+01   .58712-03   -.50251+06   .61372+02  1000.  2500.    HO
    HO2         33.008
 .50000+04   .36387+05   .82485+01   .32199-02   -.82934+05   .81654+02   300.  1000.    HO2
 .50000+04   .32593+05   .12102+02   .54010-03   -.12571+07   .80006+02  1000.  2500.    HO2
    CH3         15.035
 .34820+05   .48677+05   .80457+01   .60835-02   -.58069+05   .81068+02   300.  1000.    CH3
 .34820+05   .42779+05   .15742+02   .12359-02   -.29064+07   .78562+02  1000.  2500.    CH3
    CH2O        30.027
-.27700+05   .54354+05   .68621+01   .80908-02   -.82595+05   .89490+02   300.  1000.    CH2O
-.27700+05   .43898+05   .17110+02   .85504-03   -.30943+07   .84938+02  1000.  2500.    CH2O
    CHO         29.019
-.29000+04   .37003+05   .74602+01   .38023-02   -.33115+05   .80992+02   300.  1000.    CHO
-.29000+04   .32424+05   .12304+02   .49109-03   -.15653+07   .79009+02  1000.  2500.    CHO
```

```
                    * KINETIC REACTION DATA *

          NUMBER OF REACTIONS= 29

 M              REACTION                         PRE EXP FACTOR  TEMP EXP      ACTIVATION        INDIVIDUAL THIRD BODY EFFIC.
                                                  (MOLE-CM-S)                  (KCAL/MOLE)       NAME1       ETB1  NAME2      ETB2

  1   CH4 +     +M   --=    CH3 +H                .1500+19+ 0.      .000       100.0000                      .000             .000
  2   CH4 +HO   +    --=    CH3 +H20              .1000+14+ 0.      .000         6.0000                      .000             .000
  3   CH4 +H    +    --=    CH3 +H2               .2000+15+ 0.      .000        11.9000                      .000             .000
  4   CH4 +0    +    --=    CH3 +HO               .2000+14+ 0.      .000         6.9000                      .000             .000
  5   CH3 +0    +    --=    CH20+H                .3500+14+ 0.      .000         3.3000                      .000             .000
  6   CH3 +02   +    --=    CH20+HO               .1000+13+ 0.      .000        15.0000                      .000             .000
  7   CH20+     +M   --=    CO  +H2               .2000+17+ 0.      .000        35.0000                      .000             .000
  8   CH20+HO   +    --=    CHO +H20              .2500+14+ 0.      .000         1.0000                      .000             .000
  9   CH20+0    +    --=    CHO +HO               .3000+14+ 0.      .000          .0000                      .000             .000
 10   CH20+H    +    --=    CHO +H2               .1700+14+ 0.      .000         3.0000                      .000             .000
 11   CHO +02   +    --=    CO  +H02              .3000+14+ 0.      .000          .0000                      .000             .000
 12   CHO +HO   +    --=    CO  +H20              .1000+15+ 0.      .000          .0000                      .000             .000
 13   CHO +0    +    --=    CO  +HO               .5400+12+ 0.      .500          .0000                      .000             .000
 14   CHO +     +M   --=    CO  +H                .2000+13+ 0.      .500        28.8000                      .000             .000
 15   CO  +HO   +    --=    C02 +H                .5500+12+ 0.      .000         1.0800                      .000             .000
 16   CO  +0    +M   --=    C02 +                 .3600+19+ 0.    -1.000         2.5000                      .000             .000
 17   H02 +0    +    --=    02  +HO               .2500+14+ 0.      .000          .0000                      .000             .000
 18   H02 +HO   +    --=    02  +H20              .2500+14+ 0.      .000          .0000                      .000             .000
 19   H02 +H    +    --=    HO  +HO               .2500+15+ 0.      .000         2.0000                      .000             .000
 20   HC2 +H    +    --=    02  +H2               .2500+14+ 0.      .000          .0000                      .000             .000
 21   H   +02   +M   --=    H02 +                 .2000+16+ 0.      .000          .8700          H2D       20.000             .000
 22   H   +02   +    --=    HO  +0                .2200+15+ 0.      .000        16.8000                      .000             .000
 23   0   +H2   +    --=    HO  +H                .1700+14+ 0.      .000         9.4600                      .000             .000
 24   HO  +H2   +    --=    H20 +H                .2200+14+ 0.      .000         5.2000                      .000             .000
 25   HO  +HO   +    --=    H20 +0                .6000+13+ 0.      .000          .7800                      .000             .000
 26   H   +HO   +M   --=    H20 +                 .7000+20+ 0.    -1.000          .0000                      .000             .000
 27   0   +H    +M   --=    HO  +                 .4000+19+ 0.    -1.000          .0000                      .000             .000
 28   H   +H    +M   --=    H2  +                 .2000+20+ 0.    -1.000          .0000                      .000             .000
 29   0   +0    +M   --=    02  +                 .4000+19+ 0.    -1.000          .0000                      .000             .000
```

```
                    * GRID INFORMATION SUMMARY TABLE *

ITERATION=   1        NUMBER OF GRID POINTS=   6


 GRID COORDINATES(CM)

  .00000     .00000      .00000      .00000      .00000      .00000

 NONDIMENSIONAL GRID INCREMENTS
  .10000+01   .10000+01   .10000+01   .10000+01   .10000+01   .10000+01

 TIME(SEC)

  .00000     .46798-01   .23452-01   .11768-01   .56849-02   .28728-02

 ENTHALPY(CAL/GM)

  .83946+02   .83946+02   .83946+02   .83944+02   .83945+02   .83945+02

 TEMPERATURE(K)

  .70000+03   .14033+04   .14000+04   .13946+04   .13853+04   .13699+04

 DENSITY(GM/CM3)

  .16848-02   .84018-03   .84208-03   .84513-03   .85052-03   .85960-03

 SYSTEM MOLECULAR WEIGHT

  .28462+02   .28456+02   .28452+02   .28446+02   .28436+02   .28420+02
```

```
                    * MOLE FRACTIONS OF  14  SPECIES *

 CH4

   .30500-01    .80940-04    .12704-03    .20056-03    .33130-03    .55747-03
 O2

   .20370+00    .14296+00    .14315+00    .14346+00    .14404+00    .14503+00
 CO2

   .10000-08    .30094-01    .29841-01    .29426-01    .28678-01    .27424-01
 H2O

   .10000-08    .60649-01    .60479-01    .60218-01    .59771-01    .59034-01
 H2

   .10000-08    .38795-04    .62602-04    .10172-03    .17241-03    .29251-03
 CO

   .10000-08    .29565-03    .48286-03    .79347-03    .13562-02    .22948-02
 CH3

   .10000-08    .21772-04    .37218-04    .61793-04    .10393-03    .17285-03
 CH2O

   .10000-08    .29325-06    .58945-06    .11943-05    .25667-05    .54839-05
 CHO

   .10000-08    .32345-09    .82067-09    .20790-08    .55306-08    .13720-07
 HO2

   .10000-08    .34452-05    .53221-05    .81628-05    .12768-04    .19605-04
 H

   .10000-08    .14966-05    .28405-05    .53078-05    .10009-04    .17405-04
 O

   .10000-08    .32907-04    .49037-04    .71534-04    .10258-03    .13398-03
 HO

   .10000-08    .20126-03    .24218-03    .28703-03    .33452-03    .36795-03
 N2

   .76580+00    .76562+00    .76552+00    .76536+00    .76509+00    .76465+00
```

7.5 Sample Problem 5 - Catalytic Combustor Fuel Conversion Efficiency

This sample problem demonstrates the PROF code plug-flow reactor and wall heat and species loss options. The problem consists of 530°K, 200 percent theoretical air methane/air mixture flowing into a monolithic catalytic combustor with 0.16cm radius channels. The interior surfaces of these channels are coated with a catalyst material which helps convert fuel and air to combustion products. The special input needed for this option is the transfer coefficient, wall temperature and gas composition at the wall. These quantities are given in the input card and output listings. A constant Nusselt number case is specified by inputting a value of one for both the Reynolds and Schmidt number exponents. The transfer coefficient parameter then becomes the mean Nusselt number divided by the hydraulic diameter squared. This is the number 40 which appears on the output listing. Following this output, the wall species concentrations are printed in the same order as the initial concentrations. Wall species concentrations and temperature are assigned at values characteristic of fully combusted inlet gases at equilibrium and with no heat loss.

The final summary output shows that most of the fuel has been converted to products within the combustor. This conversion of fuel is due solely to wall reactions since the homogeneous reactions have remained inactive over the length of the combustor. The activity of the reactions can be assessed by examining the major and minor species concentrations and reaction rate output for all of the grid points.

SAMPLE PROBLEM 7.5

```
  1.    CH4/AIR CAT COMB
  2.     16  0 16 25  1  0  1  1 -4  0  1  0  0  2  0  0
  3.      14.       0.        1.        530.      0.        0.
  4.    1.        1.        1.        1.        1.        1.        1.        1.
  5.    1.        1.        1.        1.        1.        1.        1.        1.
  6.    1.        1.        1.        1.        1.        1.        1.        1.
  7.     1.
  8.     .15       .15       .15       .15       .15       .15       .15       .15
  9.     .15       .15       .2        .2        .2        .2        .2        .3
 10.    .3         .4        .4        .4        .5        .5        .5        1.
 11.     1.
 12.       1       40.
 13.       2        1410.         1.        1.
 14.          1.-9.07517     .037593  .075197         1.-9      1.-9      1.-9      1.-9
 15.          1.-9      1.-9      1.-9      1.-9      1.-9 .81204         1.-9      1.-9
 16.    CH4       .037598   .037598    1.0523
 17.    O2        .15036    .15036     1.04679
 18.    CO2             1.-9      1.-9  .8
 19.    H2O             1.-9      1.-9     1.298
 20.    H2              1.-9      1.-9 3.5333
 21.    CO              1.-9      1.-9 .9830
 22.    CH3             1.-9      1.-9   1.3257
 23.    CH2O            1.-9      1.-9 1.298
 24.    CHO             1.-9      1.-9 .9604
 25.    HO2             1.-9      1.-9  .9016
 26.    H               1.-9      1.-9 5.1557
 27.    O               1.-9      1.-9  1.4158
 28.    HO              1.-9      1.-9  1.3475
 29.    N2        .81204    .81204      .9732
 30.    N               1.-9      1.-9    1.43
 31.    NO              1.-9      1.-9 1.37
 32.    END
 33.     31
 34.    CH4  HO         CH3  H2O          1.00+13   0.0      6.000
 35.    CH4  H          CH3  H2           2.00+14   0.0     11.900
 36.    CH4  O          CH3  HO           2.00+13   0.0      6.900
 37.    CH3  O          CH2O H            3.50+13   0.0      3.300
 38.    CH3  O2         CH2O HO           1.00+12   0.0     15.000
 39.    CH2O      M     CO   H2           2.00+16   0.0     35.000
 40.    CH2O HO         CHO  H2O          2.50+13   0.0      1.000
 41.    CH2O O          CHO  HO           3.00+13   0.0      0.
 42.    CH2O H          CHO  H2           1.70+13   0.0      3.000
 43.    CHO  O2         CO   HO2          3.00+13   0.0      0.
 44.    CHO  HO         CO   H2O          1.00+14   0.0      0.
 45.    CHO  O          CO   HO           5.40+11   0.5      0.
 46.    CHO       M     CO   H            2.00+12   0.5     28.800
 47.    CO   HO         CO2  H            5.50+11   0.0      1.080
 48.    CO   O    M     CO2               3.60+18  -1.0      2.500
 49.    HO2  O          O2   HO           2.50+13   0.0      0.
 50.    HO2  HO         O2   H2O          2.50+13   0.0      0.
 51.    HO2  H          HO   HO           2.50+14   0.0      2.000
 52.    HO2  H          O2   H2           2.50+13   0.0       .000
 53.    H    O2   M     HO2               2.00+15   0.0       .870   H2O  20.
 54.    H    O2         HO   O            2.20+14   0.0     16.800
```

```
55.     O    H2            HO   H           1.70+13    0.0      9.460
56.     HO   H2            H2O  H           2.20+13    0.0      5.200
57.     HO   HO            H2O  O           6.00+12    0.0       .780
58.     H    HO    M       H2O              7.00+19   -1.0     0.
59.     O    H     M       HO               4.00+18   -1.0     0.
60.     H    H     M       H2               2.00+19   -1.0     0.
61.     O    O     M       O2               4.00+18   -1.0     0.
62.     HO   N             H    NO          4.00+13     .5      .00
63.     N    O2            NO   O           6.50+09    1.      6.30
64.     O    N2            N    NO          1.41+14     .0     75.2
```

```
                    PREMIXED ONE DIMENSIONAL FLAME CODE SOLUTION (PROF)

                  PROGRAM DOCUMENTED IN THE "PROF CODE USER'S MANUAL",
                   AEROTHERM/ACUREX CORP FINAL REPORT 78-277
                           PHONE 415/964-3200


CH4/AIR CAT COMB

                             * INTEGRAL PARAMETERS *

COLUMN                                       COLUMN
  3  NO. SPECIES CONSERVATION EQS.  16          6  PROBLEM TYPE AND ENERGY EQ.      0
  9  NO. OF SPECIES                 16         12  NO. AXIAL GRID PTS.             25
 15  NO. GRID SOLUTION ITERATIONS    1         18  SOLUTION CYCLE CONTROL NO.       0
 21  READ INITIAL MOLE FRACTION      1         24  READ NONINTEGRAL PARAMETERS      1
 27  THERMO DATA & HEAT LOSS MODEL  -4         30  CONSTRAINT SWITCH                0
 33  READ KINETIC DATA               1         36  CONSTRAINT APPLIED TO VARIABLE   0
 39  CONSTRAINT APPLIED TO GRID PT.  0         42  OUTPUT CONTROL NO.               2
 45  FLAMEHOLDER TEMP ASSIGN SWITCH  0         48  INPUT MASS FLOWRATE SWITCH       0


                             * NONINTEGRAL PARAMETERS *

 APR=DEL/MCOT= .14000+02   BP=DBAR/(DEL*MDOT)= .00000       P=   1.000(ATM)   TI=   530.0(K)

     TKAF=    .00000   TFLAME=     .0(K)


                             * GRID PARAMETERS *

  A(N)**2 ,N=1, 25

  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
       .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01  .1000+01
            .1000+01  .1000+01  .1000+01  .1000+01  .1000+01

  SIGMA(N),N=1, 25

  .1500+00  .1500+00  .1500+00  .1500+00  .1500+00  .1500+00  .1500+00  .1500+00  .1500+00  .1500+00
       .2000+00  .2000+00  .2000+00  .2000+00  .2000+00  .3000+00  .3000+00  .4000+00  .4000+00  .4000+00
            .5000+00  .5000+00  .5000+00  .1000+01  .1000+01
```

```
                           * HEAT LOSS DATA *

NO. OF STATIONS=   1        QLS= .40000+02

     REACTIVITY PAR= 2    WALL TEMP= .14100+04

     REYNOLDS EXPONENT = .10000+01     SCHMIDT EXPONENT = .10000+01

WALL SPECIES CONCENTRATIONS

 .10000-08 .75170-01 .37593-01 .75197-01 .10000-08 .10000-08 .10000-08 .10000-08
                .10000-08 .10000-08 .10000-08 .10000-08 .10000-08 .81204+00 .10000-08 .10000-08
```

```
                    * GRID INFORMATION SUMMARY TABLE *


ITERATION=   1       NUMBER OF GRID POINTS=  25


 GRID COORDINATES(CM)

  .00000      .15000+00   .30000+00   .45000+00   .60000+00   .75000+00   .90000+00   .10500+01
       .12000+01   .13500+01   .15000+01   .17000+01   .19000+01   .21000+01   .23000+01   .25000+01
            .28000+01   .31000+01   .35000+01   .39000+01   .43000+01   .48000+01   .53000+01   .58000+01
                 .68000+01

NONDIMENSIONAL GRID INCREMENTS
  .15000+00   .15000+00   .15000+00   .15000+00   .15000+00   .15000+00   .15000+00   .15000+00
       .15000+00   .15000+00   .20000+00   .20000+00   .20000+00   .20000+00   .20000+00   .30000+00
            .30000+00   .40000+00   .40000+00   .40000+00   .50000+00   .50000+00   .50000+00   .10000+01
                 .10000+01

TIME(SEC)

  .00000      .12044-02   .21683-02   .29950-02   .37352-02   .44169-02   .50576-02   .56683-02
       .62568-02   .68284-02   .73864-02   .81149-02   .88313-02   .95389-02   .10240-01   .10936-01
            .11973-01   .13005-01   .14376-01   .15744-01   .17110-01   .18816-01   .20521-01   .22226-01
                 .25635-01

ENTHALPY(CAL/GM)

  .35202+02   .35035+02   .35160+02   .35447+02   .35793+02   .36128+02   .36407+02   .36609+02
       .36728+02   .36767+02   .36720+02   .36574+02   .36364+02   .36116+02   .35848+02   .35512+02
            .35135+02   .34754+02   .34400+02   .34124+02   .33895+02   .33718+02   .33596+02   .33491+02
                 .33422+02

TEMPERATURE(K)

  .53000+03   .68649+03   .81871+03   .92870+03   .10193+04   .10936+04   .11542+04   .12036+04
       .12436+04   .12761+04   .13058+04   .13314+04   .13508+04   .13655+04   .13765+04   .13863+04
            .13942+04   .14000+04   .14040+04   .14064+04   .14079+04   .14089+04   .14094+04   .14097+04
                 .14099+04

DENSITY(GM/CM3)

  .64761-03   .49945-03   .41852-03   .36885-03   .33604-03   .31327-03   .29687-03   .28477-03
       .27567-03   .26872-03   .26269-03   .25769-03   .25404-03   .25135-03   .24936-03   .24762-03
            .24623-03   .24521-03   .24451-03   .24409-03   .24381-03   .24364-03   .24355-03   .24348-03
                 .24345-03

SYSTEM MOLECULAR WEIGHT

  .28165+02   .28135+02   .28117+02   .28109+02   .28108+02   .28111+02   .28117+02   .28124+02
       .28132+02   .28139+02   .28146+02   .28153+02   .28159+02   .28163+02   .28166+02   .28168+02
            .28169+02   .28170+02   .28169+02   .28169+02   .28168+02   .28167+02   .28166+02   .28165+02
                 .28165+02
```

```
                    * MOLE FRACTIONS OF  16  SPECIES *


CH4

  .37598-01   .31466-01   .26094-01   .21492-01   .17610-01   .14370-01   .11689-01   .94830-02
      .76778-02   .62059-02   .48526-02   .36737-02   .27777-02   .20982-02   .15837-02   .11254-02
          .75526-03   .48012-03   .28987-03   .17489-03   .10048-03   .55097-04   .30205-04   .13505-04
              .50982-05
O2

  .15036+00   .13807+00   .12732+00   .11812+00   .11036+00   .10390+00   .98548-01   .94151-01
      .90552-01   .87618-01   .84920-01   .82567-01   .80778-01   .79419-01   .78388-01   .77467-01
          .76721-01   .76164-01   .75776-01   .75540-01   .75385-01   .75290-01   .75237-01   .75201-01
              .75182-01
CO2

  .10000-08   .48179-02   .92277-02   .13180-01   .16673-01   .19727-01   .22377-01   .24662-01
      .26624-01   .28302-01   .29931-01   .31438-01   .32654-01   .33633-01   .34420-01   .35173-01
          .35832-01   .36368-01   .36776-01   .37049-01   .37245-01   .37379-01   .37461-01   .37525-01
              .37563-01
H2O

  .10000-08   .14480-01   .26706-01   .36787-01   .44964-01   .51518-01   .56726-01   .60835-01
      .64060-01   .66580-01   .68788-01   .70611-01   .71922-01   .72863-01   .73537-01   .74099-01
          .74519-01   .74806-01   .74986-01   .75084-01   .75141-01   .75171-01   .75185-01   .75193-01
              .75196-01
H2

  .10000-08   .12628-08   .15542-08   .30260-08   .58225-08   .86103-08   .11428-07   .14623-07
      .18729-07   .24712-07   .36258-07   .58184-07   .90019-07   .13018-06   .17459-06   .22765-06
          .27480-06   .29747-06   .28369-06   .24230-06   .18408-06   .12549-06   .81068-07   .43317-07
              .21208-07
CO

  .10000-08   .19971-08   .21823-08   .41340-08   .85799-08   .14039-07   .20400-07   .28016-07
      .37653-07   .50888-07   .75073-07   .12075-06   .18947-06   .28176-06   .39276-06   .54396-06
          .71042-06   .84460-06   .89665-06   .85549-06   .73577-06   .57240-06   .41847-06   .25172-06
              .12686-06
CH3

  .10000-08   .63925-08   .70793-08   .78500-08   .86916-08   .95753-08   .10607-07   .12080-07
      .14531-07   .18761-07   .27383-07   .43194-07   .64591-07   .89358-07   .11420-06   .14038-06
          .15899-06   .16126-06   .14392-06   .11519-06   .81829-07   .51980-07   .31183-07   .14890-07
              .58900-08
CH2O

  .10000-08   .12179-08   .19209-08   .20356-08   .11057-08   .54233-09   .33387-09   .24987-09
      .21901-09   .22148-09   .26075-09   .34369-09   .45047-09   .56533-09   .67201-09   .77525-09
          .83474-09   .81580-09   .70990-09   .55978-09   .39406-09   .24917-09   .14936-09   .71645-10
              .28864-10
CHO

  .10000-08   .15251-13   .37425-14   .54097-14   .71920-14   .89991-14   .10759-13   .12417-13
      .13936-13   .15296-13   .16658-13   .17952-13   .19031-13   .19947-13   .20747-13   .21616-13
          .22511-13   .23332-13   .23904-13   .24082-13   .23932-13   .23589-13   .23246-13   .22903-13
```

```
              .22674-13
 HO2

    .10000-08   .32184-08   .34175-08   .34312-08   .33610-08   .32611-08   .32162-08   .34113-08
          .41033-08   .54773-08   .79158-08   .11259-07   .14573-07   .17468-07   .19806-07   .21926-07
                .23606-07   .24796-07   .25552-07   .25954-07   .26167-07   .26265-07   .26301-07   .26315-07
                      .26318-07
 H

    .10000-08   .22733-10   .98715-11   .78217-11   .66144-11   .60700-11   .60641-11   .66286-11
          .81122-11   .11304-10   .18397-10   .31494-10   .48841-10   .68172-10   .87299-10   .10822-09
                .12826-09   .14530-09   .15805-09   .16557-09   .16950-09   .17078-09   .17070-09   .17002-09
                      .16937-09
 O

    .10000-08   .33909-10   .71705-11   .76474-11   .91341-11   .11173-10   .13906-10   .17750-10
          .23830-10   .34765-10   .58968-10   .10803-09   .18144-09   .27321-09   .37359-09   .49420-09
                .62094-09   .73993-09   .84127-09   .91368-09   .96569-09   .99823-09   .10150-08   .10245-08
                      .10279-08
 HO

    .10000-08   .56076-10   .26841-10   .48864-10   .86569-10   .14370-09   .23041-09   .37105-09
          .62092-09   .10942-08   .22107-08   .48423-08   .98158-08   .18161-07   .30805-07   .53117-07
                .88900-07   .14009-06   .20381-06   .26547-06   .32246-06   .36726-06   .39600-06   .41694-06
                      .42770-06
 N2

    .81204+00   .81117+00   .81066+00   .81042+00   .81039+00   .81049+00   .81066+00   .81087+00
          .81109+00   .81129+00   .81151+00   .81171+00   .81187+00   .81199+00   .81207+00   .81213+00
                .81217+00   .81218+00   .81217+00   .81215+00   .81213+00   .81210+00   .81209+00   .81207+00
                      .81205+00
 N

    .10000-08   .11044-10   .15605-11   .12173-11   .10877-11   .10270-11   .99888-12   .98767-12
          .98540-12   .98780-12   .99322-12   .10004-11   .10073-11   .10134-11   .10184-11   .10231-11
                .10267-11   .10291-11   .10303-11   .10306-11   .10304-11   .10301-11   .10299-11   .10297-11
                      .10296-11
 NO

    .10000-08   .19955-08   .20111-08   .20169-08   .20217-08   .20258-08   .20293-08   .20321-08
          .20345-08   .20364-08   .20381-08   .20396-08   .20407-08   .20415-08   .20420-08   .20424-08
                .20427-08   .20429-08   .20430-08   .20429-08   .20429-08   .20429-08   .20428-08   .20428-08
                      .20428-08
```

SECTION 8

DEBUG OUTPUT AND PROBLEMS AND PITFALLS

This section discusses the output which is printed when the chemistry routine fails to converge in the allotted number of iterations. This debug output does not signal the end of a solution attempt. Rescue procedures are built into the code which allows the chemistry routine to converge on one or more intermediate solutions before proceeding to the solution of interest. Through this procedure, first guesses are sequentially improved until it becomes an easy matter to converge to the solution of interest.

Nonconvergences and the resulting debug output are typically the result of bad input data and poor first guesses. Some pointers on how to avoid nonconvergences are discussed in the problems and pitfalls subsection.

8.1 Debug Output Description

The chemistry solver routine has 50 iterations in which to converge. If 47 iterations are exceeded, the routine begins to print out detailed information on the conservation equations and kinetic reaction rates. This output can also be activated by inputting a KR7 value greater than three (See Section 5.1, Card 2).

The first output to appear, listed on the following pages, gives thermochemical information for the individual species. Quantities output include molar specific heat, enthalpy, and partial and log partial pressure. The next group of output gives information on the errors in the equations and the derivatives of the change in equation error with respect to the change in the variables. This output is headed by the iteration number. Following this output, the equation error and derivatives of equation errors with respect to the log of the variables are printed out. This information, labeled A(I,J), R(I), is arranged in the following matrix form:

$$\begin{array}{l|ccccc||c|}
 & \ell nT & \ell nPM & \ell np_1 & \ell np_2 \;.. & \ell np_{IS} & \text{Error} \\
\text{Enthalpy} & & & & & & \\
\text{Sum of partial pressures} & & \dfrac{\partial E_i}{\partial V_j} & & & & E_i \\
\text{Species 1} & & & & & & \\
\text{Species 2} & & & & & & \\
\vdots & & & & & & \\
\text{Species IS} & & & & & &
\end{array}$$

where E_i represents the equation error and V_j is the log of the variable. The effects of kinetics have not yet been included in these equations and derivatives. Recalling the discussion in Section 4.1.2, after the addition of kinetics to the above matrix, the chemistry routine determines the needed corrections to the present solution estimates by inverting the matrix and multiplying by the equation errors. Examining these derivatives and errors prior to inversion can give useful insights into solution problems. Also comparison of the matrix and errors before and after kinetics indicates the importance of kinetics on the solution.

The BIG(N) output gives the biggest positive or negative term found in each species equation. The kinetic contribution to the equation is compared to this term to establish if kinetics is dominating the equations. If kinetics is dominating, the group of equations will be rearranged so as to introduce the kinetics into only one equation.

The PRMU, M, etc. output appears for each kinetic reaction. The first lines of numbers are the PRMU values which are the product of the time or space step parameter and the reaction stoichiometric coefficients. The order of PRMU is the same as the species concentration input. The line of output beginning with an integer, which is the reaction number, gives detailed information on reaction rates. FKF and PPX are the log of the reaction rate constant coefficient and the third body rate coefficient multiplier respectively. SUMK and SUMR, when combined with VLK, give the backward and forward rates of the reaction. These are printed out as PKP and PKR respectively. The difference between these rates is the net reaction rate, PMR. EXK and EAK are the same quantities as defined in the input.

The second BIG(N) output gives the largest positive term followed by the largest negative term found in the species equations after the addition of kinetics. Comparison of this output with the first BIG(N) output indicates the significance of kinetics on the equations.

The LL(I) output indicates if specific dominating reactions have been assigned to the mass balances. Zero indicates that no specific reaction has been assigned and a negative sign indicates that the mass balance has been reconfigured to behave like an equilibrium equation.

The MA(L) output gives the order of the reactions from fast to slow. The fast reactions will dominate the solution behavior.

The second A(I,J), RHS(I) output gives the derivatives matrix and equation errors after kinetics have been added to the solution. Comparison of this matrix and errors with those printed out before the addition of kinetics indicates the impact of kinetics on the solution. This matrix of derivatives is inverted and multiplied by the equation errors to obtain the corrections to the variables.

The final A(I,J) and RHS(I) outputs are the partial matrix inverse of the above-mentioned A(I,J) and the log of the corrections to the variables, respectively. The relative magnitude of the corrections with respect to the variables indicates how close the solution is to convergence. When the relative corrections become less than 0.00001 the solution procedure is converged.

The DAMP, T and PM output are the correction multiplier, temperature in °K and pressure molecular weight product in atmosphere-gm-mole units respectively. The DAMP multiplying factor is used when the corrections exceed built-in limits on the percent of variable increase or decrease per iteration. The multiplying factor is applied uniformly to all variable corrections. DAMP typically starts out less than one and approaches one as the solution converges. Values of DAMP much less than one indicate that the solution is far from convergence.

Output following DAMP, T and PM is the log partial pressure of the species concentrations listed in the same order as the input species concentrations.

The "allowed iterations exceeded" output indicates that the solution has failed to converge in 50 iterations and the time or space step has been cut by a factor of 2, as indicated by IB = 2. Cutting the time or space step by a factor of 2 (or more for subsequent nonconvergences) allows the solution procedure to converge on a more easily obtained intermediate solution before proceeding to the solution of interest. However, if the time or space step is cut by a factor of 256 and the solution still has not converged, it is then assumed that a serious problem exists and the solution procedure is terminated.

8.2 Flame Solution, Problems and Pitfalls

The PROF code flame option treats problems which are steady in time. Transient problems, such as flames being extinguished at the flameholder or "blown off" the burner, are not handled by the code. If the code is given poor flame speed parameter or species concentrations first guesses, these unsteady solutions might be sought by the code. In these cases the final result will be a prediction of unburnt gas or the trivial unignited flame case. To avoid these solutions, some care must be taken in developing first guess input data.

To maximize the probability of convergence to a hot solution, always use downstream stable species guesses which are characteristic of the burnt gas mixture. These can be guessed at or they can be scaled from a prior solution. If punched card output from a prior solution is input, make sure that there are no discontinuities in concentrations from the initial point to the first grid station. If punched cards are not used for first guesses, input downstream unstable species concentrations characteristic of the maximum values which are found in the flame. These first guess concentrations will help "light off" the flame.

First guess values for the flame speed parameter must also be carefully chosen. Large and small values of the parameter relative to the correct value, will lead to extinction and blowoff respectively. An estimate of flame speed should be used to calculate the flame speed parameter. Large values of DAPR relative to APR indicate that either poor guesses for APR or species concentrations have been input into the code. If this type of output persists for several iterations, along with small damp valves, then the first guesses should be carefully reviewed and revised as needed. The constraint condition should also be examined at this time.

To maximize the probability of convergence, the constraint condition should be applied to a monotonically increasing or decreasing species concentration in a region where the concentration is changing rapidly. A value between one-third and two-thirds of the maximum value found within the flame is suggested. A stable species which represents a sizeable fraction of the total gas is a good candidate for the constraint variable.

The solution procedure, being fully implicit in nature, does not have any limitations on step size or grid spacing. However, for accurate results, grid spacings must be made sufficiently small to define species gradients. Problems arise when step sizes are too large and the "flame zone" is captured within one grid spacing. These cases will have very large errors. For free flame cases, grid spacings near the constraint condition should be on the order of one-tenth of the values at the upstream and downstream boundaries. This distribution of grid spacings should give adequate gradient resolution over the entire flame length. For flames attached to flameholders, gradients at the upstream boundary near the flameholder, are substantial and small grid spacings should be applied from the upstream boundary through to the constraint location. Downstream of the constraint, larger grid spacings can be applied without adversely affecting accuracy.

Once the solution is converged, the adequacy of the selected grid spacings can be assessed and needed revisions can be made to the grid spacings.

It should be noted that many free flame calculations have been made with the PROF code using crude first guesses. Nearly all of these cases converged to hot flames. When the solution did not converge, it was typically because extremely poor first guesses were input. Therefore, some care in input preparation should be exercised to maximize the probability of convergence.

8.3 Well-Stirred, Plug-Flow and Time-Evolution Chemical Kinetic Solution Problems and Pitfalls

The PROF nonflame code options employ the flame chemistry routine with simple driver logic to either march in space or time. Problems encountered with these options are typically associated with the chemistry routine not receiving adequate first guesses for temperature (where applicable) and species concentrations. Since the upstream conditions are used as first guesses in these marching procedures, the solution problems are associated with taking too large a time or space step. Simply reducing the step size will alleviate the problem in most cases.

For the well-stirred reactor option the time step is large and fixed. This can lead to solution problems. However, first guesses to the solution can be sequentially improved by converging on a number of easily obtained well-stirred reactor solutions. The solution at the last reactor time step is used as the first guess for the current reactor solution. By this procedure the code can "creep" to the solution of interest.

Well-stirred reactor initial conditions are usually cold and unreacted. To ensure "ignition" of the reactor, a temperature characteristic of the burnt gas should be inserted in the TFLAME input (See Section 5.1, input card set 3). This input is used as the temperature first guess for the solution of interest.

The well-stirred reactor solution procedure has the greatest difficulty when the reactor time constant is near the blowout limit. Starting with poor first guesses, solution excursions during intermediate iterations can result in nonconvergences. To improve first guesses in these cases, a sequence of solutions should be carried out, starting from the easily obtained near equilibrium case (i.e. very large time step). As the blowout limit is approached the difference in reactor time constants between solutions should be reduced. Solutions for intermediate and final time constants of interest should be achievable by this approach.

8.1 SAMPLE DEBUG OUTPUT

```
CPF.HI.SB.TC.E.PP
     CH4        .2038+02 -.5763+03  .5048+02  .2027+00  .5068+02  .3094-07 -.1729+02
     O2         .8691+01  .9108+04  .3157+02 -.3204+01  .2836+02  .4805+00 -.7330+00
     CO2        .1387+02 -.8025+05  .3702+02  .2823+02  .6524+02  .1116+00 -.2193+01
     H2O        .1110+02 -.4705+05  .3144+02  .1655+02  .4799+02  .2097+00 -.1562+01
     H2         .7655+01  .8149+04  .3604+02 -.2866+01  .3318+02  .4051-06 -.1472+02
     CO         .7998+01 -.1779+05  .3933+02  .6259+01  .4559+02  .6236-04 -.9683+01
     CH3        .1609+02  .4967+05  .5614+02 -.1747+02  .3867+02  .8737-10 -.2316+02
     CH2O       .1682+02 -.1248+05  .5376+02  .4391+01  .5815+02  .1943-07 -.1776+02
     CHO        .1224+02  .9087+04  .5344+02 -.3196+01  .5025+02  .9291-08 -.1849+02
     HO2        .1226+02  .1719+05  .5509+02 -.6046+01  .4904+02  .2990-08 -.1963+02
     H          .4968+01  .5773+05  .4098+02 -.2031+02  .2068+02  .7819-10 -.2327+02
     O          .4983+01  .6526+05  .4333+02 -.2295+02  .2037+02  .2131-08 -.1997+02
     HO         .7813+01  .1770+05  .4184+02 -.6227+01  .3561+02  .7936-06 -.1405+02
     N2         .8284+01  .8614+04  .2794+02 -.3030+01  .2491+02  .2606+01  .9579+00
```

```
15    .17580+02 .00000    .44789+01 -.31803+02 -.15189+02  .99617+01 -.10000+01  .10000+04  .32689-09  .37089-11  .32319-09
  .000      .000      .000      .557+09 -.557+09   .000       .000       .000       .000       .000      .557+09    .000
 -.557+09   .000
22    .26608+02 .00000   -.11882+00 -.28766+02 -.53377+01  .10246+02 -.20000+01  .52000+04  .90589-08  .10202-07 -.11429-08
  .000     -.557+09   .000      .000      .000       .000       .000       .000       .000      .557+09   -.557+09    .000
  .000      .000
21    .27518+02 .34000+01 .87261-04 -.24005+02 -.17463+02  .53676+01 -.30000+01  .10000+04  .80524-08  .80517-08  .70266-12
  .000     -.557+09  .557+09    .000      .000     -.557+09    .000       .000       .000       .000       .000      .557+09
  .000      .000
 1    .25691+02 .00000    .11667+02 -.10416+02 -.22157+01 -.99451+01 -.20000+01  .60000+05  .14371-08  .12316-13  .14371-08
  .000      .000     -.557+09   .000      .000      .557+09    .000       .000       .000       .000       .000      .557+09
  .000      .000
19    .31520+02 .34000+01 .71782+00 -.21927+01  .44922+02 -.18185+02 -.20000+01  .10000+06  .14122-08  .68888-09  .72330-09
  .000      .000      .000     -.557+09   .000       .000       .000       .000       .000       .000      .557+09    .000
  .557+09   .000
 2    .32619+02 .34000+01 .82988+01 -.15622+01  .43082+02 -.18846+02 -.20000+01  .10500+06  .13710-08  .34113-12  .13707-08
 -.557+09   .000      .000      .557+09   .000       .000      .557+09    .000       .000       .000       .000       .000
 -.557+09   .000
 5    .26790+02 .00000    .37553+00 -.31338+02 -.51035+01  .10499+02 -.20000+01  .50000+04  .89073-09  .61187-09  .27887-09
  .000      .000      .000      .000      .000       .000       .000      -.557+09   .557+09    .000       .000      -.557+09
  .557+09   .000
17    .21779+02 .00000    .73343+01 -.37723+02 -.91405+01  .12966+02 -.10000+01  .44000+04  .17694-10  .11550-13  .17682-10
  .000      .000      .000      .000      .000      .557+09    .000       .000      -.557+09    .000       .000      -.557+09
  .557+09   .000
18    .22185+02 .00000    .10573+02 -.38461+02 -.26183+02  .14743+02 -.10000+01  .50000+03  .50032-10  .12807-14  .50031-10
  .000     -.557+09   .000      .000      .000       .000      -.557+09    .557+09    .000       .000       .000       .000
  .557+09   .000
14    .26790+02 .00000    .26723+02 -.23894+02 -.18839+02  .17055+01 -.20000+01  .30000+05  .23105-09  .57313-21  .23105-09
  .000     -.557+09   .000      .000      .000       .000       .000       .000       .000       .000       .000      .111+10
  .000      .000
 4    .41647+02 .34000+01 .12385+02 -.75303+00  .42706+02 -.21903+02 -.30000+01  .11870+06  .14774-09  .61764-15  .14774-09
 -.557+09   .000      .000      .000      .000       .000      .557+09    .000       .000       .000      .557+09    .000
  .000      .000
12    .36819+02 .34000+01 .86743+01 -.17291+02  .37978+02 -.86664+01 -.20000+01  .88000+05  .53305-11  .91107-15  .53296-11
  .000      .000      .000      .000      .557+09    .000       .000      -.557+09   .557+09    .000      -.557+09    .000
  .000      .000
16    .19007+02 .00000    .45977+01 -.41028+02 -.98517+01  .10615+02 -.10000+01  .32000+04  .61895-13  .62359-15  .61271-13
  .000      .000      .000      .000      .557+09    .000       .000       .000       .000       .000      -.557+09   .557+09
 -.557+09   .000
 8    .18561+02 .00000   -.27365+01 -.37319+02 -.71117+00  .88322+01 -.10000+01  .70000+04  .42514-12  .65614-11 -.61362-11
 -.557+09   .000      .000      .000      .000       .000      .557+09    .000       .000       .000       .000      -.557+09
  .557+09   .000
10    .18784+02 .00000    .32309+01 -.37258+02  .94531+00  .87036+01 -.10000+01  .80000+04  .39713-12  .15695-13  .38143-12
  .000      .000      .000      .000      .000       .000       .000       .000       .000      -.557+09   -.557+09    .000
  .111+10   .000
 9    .28910+02 .00000    .14981+01 -.42900+02 -.13897+02  .13710+02 -.20000+01  .19000+04  .21027-12  .47008-13  .16327-12
 -.557+09   .000      .000      .000      .557+09    .000      .557+09    .000       .000       .000      -.557+09    .000
  .000      .000
11    .20393+02 .00000    .49435+00 -.40563+02  .23414+00  .96095+01 -.10000+01  .10000+05  .36061-13  .21996-13  .14065-13
  .000      .000      .000      .000      .000       .000      -.557+09    .557+09    .000       .000      .557+09   -.557+09
  .000      .000
13    .24082+02 .00000    .19781+02 -.43128+02 -.24511+02  .13288+02 -.15000+01 -.30000+03  .10985-12  .28188-21  .10985-12
  .000      .000      .000      .000     -.557+09    .000       .000       .000       .000       .000      .111+10    .000
  .000      .000
 3    .29911+02 .34000+01 .81800+01 -.14719+02  .37744+02 -.18388+02 -.20000+01  .96000+05  .41858-14  .11729-17  .41846-14
 1  6 .3243-06
12  0 .5570+09  .3403-08 -.2131-08
```

```
ITERATION 49
 RHS1,RHS2,E,I=1,IS
   .130+03  -.795-02   .104+00   .213+00  -.112+00  -.210+00  -.402-06  -.624-04   .332-08  -.160-07
  -.589-08   .413-09   .332-08   .127-08  -.790-06  -.125-05
A(I,J),RHS(I),BEFORE
  .4242+05 -.8131+04 -.1783-04  .4376+04 -.8957+04 -.9866+04  .3301-02 -.1110+01  .4340-05 -.2426-03  .8442-04  .5140-04
   .4514-05  .1390-03  .1405-01  .2245+05  .1305+03
  .0000     .0000     .3094-07  .4805+00  .1116+00  .2097+00  .4051-06  .6236-04  .8737-10  .1943-07  .9291-08  .2990-08
   .7819-10  .2131-08  .7936-06  .2606+01 -.7952-02
  .0000    -.1038+00  .3094-07  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .0000     .1038+00
  .0000    -.6932+00  .0000     .4805+00  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .0000     .2128+00
  .0000    -.3403-08  .0000     .0000     .1116+00  .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .0000    -.1116+00
  .0000    -.3403-08  .0000     .0000     .0000     .2097+00  .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .0000    -.2097+00
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .4051-06  .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .0000    -.4017-06
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .6236-04  .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .0000    -.6236-04
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .8737-10  .0000     .0000     .0000
   .0000     .0000     .0000     .0000     .3316-08
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .1943-07  .0000     .0000
   .0000     .0000     .0000     .0000    -.1603-07
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .9291-08  .0000
   .0000     .0000     .0000     .0000    -.5888-08
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .2990-08
   .0000     .0000     .0000     .0000     .4131-09
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .7819-10  .0000     .0000     .0000     .3325-08
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .2131-08  .0000     .0000     .1273-08
  .0000    -.3403-08  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .7936-06  .0000    -.7902-06
  .0000    -.2606+01  .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000     .0000
   .0000     .0000     .0000     .2606+01 -.1252-05
BIG(I),I=1,IS  .1038+00  .6932+00  .3403-08  .3403-08  .3403-08  .3403-08  .3403-08  .3403-08  .3403-08  .3403-08
BIG(I),I=1,IS  .3403-08  .3403-08  .3403-08  .2606+01 -.3094-07 -.4805+00 -.1116+00 -.2097+00 -.4051-06 -.6236-04
BIG(I),I=1,IS -.8737-10 -.1943-07 -.9291-08 -.2990-08 -.7819-10 -.2131-08 -.7936-06 -.2606+01

PRMU,M,FKF,PPX,SUMK,SUMR,DKPT,VLK,EXK,EAK,PKR,PKP,PMR

   .000      .557+09   .000       .000       .000       .000       .000       .000       .000       .000       .557+09  -.557+09
  -.557+09   .000
 7     .26608+02  .00000     -.69416+01 -.34014+02 -.56728+01  .12075+02 -.20000+01  .00000     .29671-09  .30693-06 -.30663-06
   .000      .000       .000       .557+09   .000       .000       .000       .000       .000       .000       .000       .557+09
  -.111+10   .000
 6     .25181+02  .00000     -.28554+01 -.28093+02 -.60489+01  .10296+02 -.20000+01  .10000+04  .18660-07  .32432-06 -.30566-06
   .000      .000       .557+09    .000       .000      -.557+09    .000       .000       .000       .000       .557+09    .000
  -.557+09   .000
20     .17867+02  .00000      .47256+01 -.23729+02 -.78886+01  .69680+01 -.15000+01  .00000     .52567-07  .46602-09  .52101-07
   .000      .000       .000       .557+09    .000       .557+09    .000       .000      -.557+09    .000       .000       .000
  -.557+09   .000
23     .19882+02  .00000      .77176+01 -.32541+02 -.32232+02  .12616+02 -.10000+01  .00000     .22220-08  .98861-12  .22210-08
   .000      .000       .000       .557+09    .000       .000       .000      -.557+09    .557+09    .000       .000       .000
  -.557+09   .000
 2  7  .3069-06
11  0  .5570+09  .3403-08 -.7819-10
 3 20  .5257-07
 6  0 -.5570+09  .3403-08 -.6236-04
 4 22  .1020-07
 5  0 -.5570+09  .3403-08 -.4051-06
 5 21  .8052-08
10  0  .5570+09  .3403-08 -.2990-08
 6 23  .2222-08
 9  0 -.5570+09  .3403-08 -.9291-08
 8 19  .1412-08
13  0  .2228+10  .1021-07 -.1247-03
10  5  .8907-09
 7  0  .5570+09  .3403-08 -.8737-10
11 15  .3269-09
 8  0 -.5570+09  .3403-08 -.1943-07
12 14  .2310-09
 1  0 -.5570+09  .1038+00 -.3094-07
BIG(I),I=1,IS  .1038+00  .6932+00  .1038+00  .2076+00  .3413-04  .1038+00  .2969-02  .1038+00  .1038+00  .3403-08
BIG(I),I=1,IS  .1038+00  .1038+00  .3054+01  .2606+01 -.6119-04 -.4805+00 -.1116+00 -.2097+00 -.3418-02 -.8004+00
BIG(I),I=1,IS -.1038+00 -.9849-02 -.2787-01 -.9094-04 -.8004+00 -.7635+00 -.3638-03 -.2606+01
          1  14  12-.3192319-12 .1991881+02 .1991881+02-.1428018-03-.2495977-01 .5721279-02
          5  22   4 .5045824+01 .1182212+00 .1991881+02 .6332159+00 .6332182+00 .9999964+00
          6  20   3-.2595752+00 .4776921+01 .4776921+01-.3056190+02-.3056577+02 .9998735+00
          7   5  10 .3408098+00 .9025544-01 .9025544-01 .3219079-01 .5472100-01 .5882713+00
          8  15  11-.2065880-02 .1176553+01 .1176553+01-.4634134-02-.8610150-01 .5362176-01
          9  23   6-.5506544-03 .7573895+01 .7573895+01-.1071412+01-.1161194+01 .9226816+00
         10  21   5 .4484808+01 .6697848-04 .6697848-04 .3004428-03 .3004428-03 .1000000+01
         11   7   2-.1652647+00 .6946163+01 .6697848-04-.1715704+03-.1715711+03 .9999963+00
         12   6   1-.1039345+02 .2859249+01 .6697848-04-.1709559+03-.1709565+03 .9999967+00
         13  19   8 .1534816+01 .1449638+01 .1449638+01 .5005916+01 .5005916+01 .9999999+00
LL(I),I=1,IS-14   0   0   0-22-20  -5-15-23-21  -7  -6-19   0
MA(I),I=1,IS   6   7  20  22  21  23   1  19   2   5  15  14   4  18  17   8  12  10   9  13  16  11   3

A(I,J),RHS(I),AFTER KINET AND BEFORE INVERT
  .4242+05 -.8131+04 -.1783-04  .4376+04 -.8957+04 -.9866+04  .3301-02 -.1110+01  .4340-05 -.2426-03  .8442-04  .5140-04
  .4514-05  .1390-03  .1405-01  .2245+05  .1305+03
 .0000     .0000     .3094-07  .4805+00  .1116+00  .2097+00  .4051-06  .6236-04  .8737-10  .1943-07  .9291-08  .2990-08
  .7819-10  .2131-08  .7936-06  .2606+01 -.7952-02
 .1097+01  .2482-01  .3094-07  .1287+00  .0000     .0000     .0000     .0000     .1288+00 -.1428-03  .0000     .0000
-.1570-12  .6119-04 -.1428-03  .0000    -.2766-01
 .0000    -.4856+00 -.6188-07  .4805+00  .0000     .0000    -.2026-06 -.3118-04 -.1529-09 -.1943-07 -.6968-08  .2243-08
-.1955-10  .1065-08  .1984-06  .0000     .5209-02
 .0000    -.1038+00  .3094-07  .0000     .1116+00  .0000     .0000     .6236-04  .8737-10  .1943-07  .9291-08  .0000
  .0000     .0000     .0000     .0000    -.7887-02
 .0000    -.2076+00  .6188-07  .0000     .0000     .2097+00  .4051-06 -.1819-11  .1311-09  .1943-07  .4645-08  .1495-08
  .3909-10  .0000     .3968-06  .0000    -.2087-02
-.3032+02 -.2697-05 -.2009-04  .0000     .0000    -.5682+01  .5683+01  .0000     .1225-04 -.3448-04  .3473-06  .0000
 -.5683+01  .3655-02  .5679+01  .0000     .6714+00
-.1956+03  .3837-02  .2969-02  .8827+00 -.3082+02  .7637+00  .2129-05  .3008+02 -.5074-06  .1943-07  .6968-08 -.1171-03
 -.3082+02 -.7549-05  .2928+02  .0000    -.1472+03
 .1847+01 -.2253-01 -.4993+00  .0000     .0000     .3730+00  .1225-04  .0000     .3730+00  .0000     .0000     .0000
 -.1958-04 -.2212-03 -.4961+00  .0000     .4353-01
-.2101+00  .8147-01  .3094-07  .0000     .0000    -.6700-02 -.3473-06  .0000     .8737-10  .1920+00 -.6707-02  .0000
  .3448-04  .9855-02  .1821+00  .0000    -.8705-01
-.3474+02  .8978-01  .3094-07  .0000     .0000    -.1072+01  .0000    -.1072+01  .8737-10  .1943-07  .1266+01  .0000
  .0000     .2787-01  .1238+01  .0000    -.8208+01
```

```
   .7832+02 -.2990-08   .0000    -.4485+01   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .4485+01
  -.4485+01   .0000    -.5237-04   .0000      .3004-03
   .9898+03   .6046-03   .3094-07   .1718+03 -.6860-05   .0000      .2026-06   .8005+00 -.6119-04   .1943-07   .6968-08   .1171-05
   .1710+03 -.1717+03 -.1717+03   .0000    -.1193+04
   .1121+04   .5684-03   .3190-02   .0000      .0000      .1814+03   .3657-02 -.7134-06 -.9250-05   .9855-02   .2786-01 -.1495-08
  -.4273-03   .1807+03 -.3627+03   .0000    -.5185+03
  -.3010+03 -.1270-03 -.1188-01 -.3292+00 -.3146+01 -.3055+01 -.8516-05   .6541+01   .2030-05   .0000      .9291-08   .4685-05
   .1231-02   .6541+01   .5514-03   .0000      .9482+01
   .0000    -.2606+01   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
   .0000      .0000      .0000      .2606+01 -.1252-05

A(I,J),RHS(I),AFTER
   .1000+01   .5292+00 -.4203-09   .1032+00 -.2112+00 -.2326+00   .7782-07 -.2616-04   .1023-09 -.5718-08   .1990-08   .1212-08
   .1064-09   .3278-08   .5312-06 -.1917+00 -.1473-01
   .0000      .1000+01   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
   .0000      .0000      .0000    -.1000+01 -.8863-03
   .0000      .0000      .1000+01   .4958+06   .7374+07   .8122+07 -.2718+01   .9136+03   .4100+07 -.4547+04 -.6950-01 -.4231-01
  -.3721-02   .1949+04 -.4559+04 -.1100+08 -.4666+01
   .0000      .0000      .0000      .1000+01   .8927+00   .9833+00 -.7253-06   .4959-04   .4964+00 -.5506-03 -.2205-07 -.7350-09
  -.4887-09   .2359-03 -.5516-03 -.2281+01   .9588-02
   .0000      .0000      .0000      .0000      .1000+01   .2297+01 -.7095-06 -.3390-03   .1160+01 -.1286-02 -.1080-06 -.1262-07
  -.1047-08   .5511-03 -.1289-02 -.1959+01 -.6842-01
   .0000      .0000      .0000      .0000      .0000      .1000+01   .3415-06 -.2774-03   .3583+00 -.3975-03 -.5265-07 -.1830-08
  -.2693-09   .1703-03 -.3979-03 -.6053+00 -.1084-01
   .0000      .0000      .0000      .0000      .0000      .0000      .1000+01   .2868-02 -.3026+01   .3352-02   .8549-06   .9554-07
  -.1000+01 -.7948-03   .1003+01 -.4158+01 -.6006+00
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .1000+01   .1337+03 -.1483+00 -.2763-04 -.7617-05
  -.1130+01   .6352-01   .9243+00   .1427+03 -.5475+01
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .1000+01 -.1110-02 -.2086-06 -.2800-07
  -.7967-03   .4752-03 -.3579-03   .1073+01 -.1030+00
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .1000+01 -.3494-01   .3281-08
   .2888-03   .5134-01   .9483+00   .4065+00 -.5585+01
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .1000+01 -.3199-05
  -.8641+00   .2202-01   .1799+01 -.1025+01 -.1604+02
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .1000+01
  -.1002+01   .2121-07   .1726-02 -.1277+01   .4104+01
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
   .1000+01 -.1000+01 -.1004+01   .9275+00   .3837+01
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
   .0000      .1000+01 -.2009+01   .9004+00   .6200+01
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
   .0000      .0000      .1000+01 -.5421+00   .4466+01
   .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000      .0000
   .0000      .0000      .0000      .1000+01 -.8868-03
DAMP=  .28709+00 T=  .14252+04 PM=  .96837+02
   -.18631+02-.73027+00-.22123+01-.15653+01-.14891+02-.11254+02-.23190+02-.19360+02-.23099+02-.18450+02
   -.22170+02-.18187+02-.12765+02 .95761+00

ALLOWED ITERATIONS EXCEEDED
FLAME PARAMETERS ITER=50   IB= 1

CPF,HI,SB,TC,E,PP
    CH4        .2027+02 -.1020+04   .4399+02   .3644+00   .4435+02   .1739-04 -.1096+02
    O2         .8677+01   .8919+04   .3149+02 -.3186+01   .2830+02   .4852+00 -.7232+00
    CO2        .1384+02 -.8055+05   .3698+02   .2877+02   .6575+02   .1037+00 -.2266+01
    H2O        .1105+02 -.4729+05   .3136+02   .1689+02   .4626+02   .2074+00 -.1573+01
    H2         .7633+01   .7982+04   .4106+02 -.2651+01   .3821+02   .2525-08 -.1980+02
```

SECTION 9

PROGRAM FORTRAN VARIABLES LIST AND DEFINITIONS

In Table 1 and 2 the common and local variables of the major routines used in the PROF code are defined. In many cases the program variable names can be related to specific variables defined in the text of this document. In other cases the terms are defined and used locally in the code for algebraic convenience. Some variable names relate to input options and are used as option flags throughout the code. All variables are included in the tables so that the user can quickly identify the nature of every variable name used. The dimensions indicated for each variable are defined at the beginning of the program list of the major routines.

TABLE 1. COMMON VARIABLES

Variable	Common	Description
A (JEX,JEZ)	F1	Basic matrix of coefficients set up in FLAME, fully inverted on last iteration in FLAME, and used to set up linearized corrections in ACEF. Equivalenced to DAA for storage economy only.
AA (JEZ,JEZ)	F3	Inverse of A loaded into AA and corrected for rearrangements in kinetics package of FLAME.
AFF (JX)	F2	Affinity of given kinetic reaction, $(= T\Delta S)$
ALA (JQ,JS)	EPRP	The "corrector" values of the species α_i's for each species at each station. They also serve as "error" variables during matrix solution of "corrector" equations.
ALB (JQ, JS)	F3	The "predictor" value of the species α_i's for each species at each station.
ALDEN (JP)	LIN	The denominator by which each term of the conservation equations (Eq. 37 and 38) is divided to produce a unity coefficient on α_{i_n} (or h_n for $i=IS+1$).
ALFW (JE)	F1	Wall values of α_i for each species.
ALPE (JQ)	F3	Guessed exit or equilibrium values of the α_i's which are input to the code. Used only to set up initial first guesses under certain options.
ALPF (JQ)	F3	Assigned initial or frozen values of the α_i's which are input to the code. These values are assigned to station one and are never varied.
ALPHI (JQ)	F1	The current set of α_i's at a given station as generated by the FLAME subroutine. Entering FLAME these variables contain the terms α_i° introduced in Eq. 44.
ALPHZ (JQ)	F3	The terms α_i° introduced in Eq. 44
AP (JS)	F3	The area ratio parameter read with card set 4. For the FLAME transformations (Eq. 36) the parameter is squared immediately after input.

TABLE 1. Continued

Variable	Common	Description
ARHM (JQ,JQ)	F3	The matrix to the right of the diagonal during the "corrector" block tridiagonal solution procedure. This matrix is set up after each FLAME computation, the diagonal matrix is solved in terms of its variable, the subsequent left-hand matrix is folded into it, and then it is stored on peripheral hardware. After completion of the last station FLAME computation, the ARHM are extracted and solved for the "corrector" α_i's starting from the last station. During the manipulation,the zero and (-1) columns of this matrix are temporarily equivalenced to the constant of the linear equations and the coefficient on a_n, respectively. (Note DUD (JQ) and DUMB (JQ) prior to ARHM (JQ,JQ) in Common list.)
AX (JS)	F4	Defined for local output of species mass fractions in ACEF.
BMU (JS)	EPRP	BMU $(\ell) = \mu_{2_{\ell+1}} - \mu_{2_\ell}$
BP	F1	Defined by Eq. 36. Input for FLAME options. Updated during iterations for assigned $\dot{m}$ option.
BPA (JQ)	F3	Defined by Eq. 36. Input for all diffusion options (axial or wall loss). Updated during iterations for assigned $\dot{m}$ option. Initially input as 1/F but immediately multipled by BP.
CHI (JS)	EPRP	Defined immediately following equation 38.
CHIW	F1	Value of $(K\mu_1/\rho\bar{D}) - \tilde{C}_p$ used in wall heat flux calculation (see Eq. 26).
CKIN (JQ)	F1	Constant coefficient on kinetic production term as developed at each station for each mass balance. Identical to CKINI (JQ) except as damped for reduced time steps prior to call of FLAME in ACEF.
CKINI (JQ)	F3	Constant coefficient on kinetic production term. (See CKIN (JQ).) This coefficient is normalized to yield unit coefficient on α_{i_n} in mass balance equation.

TABLE 1. Continued

Variable	Common	Description
CPF (JP)	F1	Molal heat capacity of each species.
CPG	F1	Heat capacity of gas mixture in cal/gm^{o}K. Within FLAME, CPG is heat capacity times PM.
CPT (JP,50)	LIN	Tabular values of molal heat capacity for each species at 100°K increments to 5000°K.
CPTIL	EPRP	Modified heat capacity $\tilde{C}_p$. Within FLAME, CPTIL is C_p times PM.
DAA (JE2,JE2)	F1	DAA (i, k) becomes the $\partial\alpha_i/\partial\alpha^o_k$ and is used for setting up corrector matrix.
DKPT (JX)	F2	The partial of log K with respect to log T for each kinetic reaction.
DQRDP (3)	F1	Partial of the emitted radiation flux per unit volume with respect to the log partial pressure CO_2, H_2O and CO, respectively.
DQRDT	F1	Partial of the emitted radiation flux per unit volume with respect to log of temperature.
DTT (JSO	F4	Elapsed times as computed from flow data.
DUD (JQ)	F3	Equals CKIN (I)* BUMP in FLAME.
DUMB (JQ)	F3	Not used.
E (JP)	F1	Prior to inversion in FLAME, equal to error of mass balance and equilibrium equations; after inversion equal to corrections in log partial pressures of species.
EAK (JX)	F2	Activation energy of kinetic reaction, cal/mole.
EGYDS	HTL	Not used.
EXK (JX)	F2	Temperature exponenet of kinetic reaction. Modified depending on nature of mass balance to include additional temperature factors multiplying kinetic production term.

TABLE 1. Continued

Variable	Common	Description
EXM	F1	Exponent m introduced after Equation 13.
EXN	F1	Exponent n introduced in Equation 13.
FKF (JX)	F2	Log of pre-exponential factor of kinetic reaction. Modified, depending on nature of mass balance, for additional multiples of the perfect gas constant. Saved in XX (JX) and then modified in each interation to include PM factors and third body terms.
FLUX (JQ)	F3	Not used.
FT	F1	Not used.
FW (JP)	F1	Difussion factor F for each species as used in wall flux relations. (Equals laminar F raised to n power.)
GT (JP,50)	LIN	Tabular values of standard state free energy function, $(G-H_{298})/T$ for each species at 100°K increments to 5000°K
H	F1	Enthalpy of gas mixture as input to FLAME. In flame solutions the parameter includes other input terms (h^o).
HBC	F1	Not used.
HH (JS)	F4	Enthalpy of gas mixture at each station (Predictor value).
HI (JP)	F1	Molal enthalpy of each species.
HOS (JP)	F1	Product of molal enthalpy and partial pressure of each species; modified to include heat transfer terms for computational efficiency.
HRF (JP)	LIN	Molal heat of formation of species at 298^oK.
HT (JP, 50)	LIN	Tabular molal enthalpy of each species relative to its value at 298^oK, given at 100^oK increments to 5000^oK.
HTCOE	EPRP	Coefficient on $\bar{h}_n$ in flame energy equation.

TABLE 1. Continued

Variable	Common	Description
HTW	F1	Value of $\tilde{h}$ at wall as in Eq. 26.
IB	F1	Counter on step size halving procedure.
ICC	F1	Value of ITC as carried by program with regard to heat loss options (see Section 5.1).
ICON	F1	Flag indicating convergence (=0) or nonconvergence (=1) of FLAME routine.
IH	F1	Index flag defining wall flux option. See page 5-8.
IQV (16,4)	LIN	Equivalent species name table (see page 5-10).
IS	F1	Number of mass balances to be considered. Same as number of species if no equilibrium reactions. (Equilibrium option inoperative.)
ISP	F1	IS+1.
ITER	F1	Iteration count in FLAME (starts at 1).
IWANT (3,JP)	WANTS	Flag (IWANT (1,J) and species name (IWANT (2&3,J)) of desired species.
KNY	LIN	Number of equivalent species name pairs to be considered (read as number of cards and multiplied by 4).
KR	F1	Kinetics flag in FLAME.
KR6	F1	Flag on solution type to be obtained (see page 5-1). Note that -1 goes to 0 and 3 goes to 2, after setting up special flags.
KR7	F1	Debug flag (see page 5-3).
L	F1	Axial station number.
MA (JX)	F2	Ordering array for kinetic equations. MA (1) is index of fastest reaction.

TABLE 1. Continued

Variable	Common	Description
MP (JX)	F2	Flag indicating those equations rearranged in FLAME to assist kinetic convergence. If MP (2) = -3 then 2nd fastest reaction was isolated into mass balance 3.
MT	F1	Number of kinetic reactions.
N	F1	Number of species.
NAMA (JP)	F1	First four characters of species name.
NAMB (JP)	F1	Second four characters of species name.
NEQ	F1	Total number of equations used in corrector step. May include T and $\tilde{h}$ equations.
NFHS	F1	Flameholder flag (NFH) as transmitted to FLAME where $L = 2$. When $L \neq 2$, NFHS = 0.
NRS (3)	F1	Indexes of CO_2, H_2O, and CO, respectively.
NWANT	WANTS	Number of species in input list. Must equal IS.
P	F1	Pressure in atmospheres.
PI (JS)	EPRP	Not used.
PKP (JX)	F2	Reverse rate of kinetic reaction.
PKR (JX)	F2	Forward rate of kinetic reaction.
PLN	F1	Log of pressure.
PLP (JP)	F1	Log of partial pressure of each species.
PML (JX,JS)	F4	Net forward rate of each reaction at each station as output.
PMR (JX)	F2	Net forward rate of each reaction as used in FLAME.
PMU (JE,JX)	F2	Stoichiometric coefficient of each product species in each reaction.

TABLE 1. Continued

Variable	Common	Description
PMW	F1	Pressure, molecular weight product at wall.
PP (JP)	F1	Partial pressure of each species.
PPI (JP)	F3	Log partial pressure of species at first station.
PPP	F1	Exponent on PM for wall flux term in mass and energy balances.
PPS (JP)	F3	Saved value of converged log partial pressure of each species used during time step halving rescue logic.
PPTC (JP)	F1	PP (I)*IC (I)
PPV	F1	Exponent on PM for volumetric heat loss term in energy balance.
PPX (JX)	F2	Third body factor for each reaction.
PRMU (JE,JX)	F2	Net stoichiometric product coefficient for each species in each reaction subsequently multiplied by CKIN (JE) for computational convenience.
PW (JP)	F1	Partial pressure of each species at the wall.
Q (JS)	HTL	Normalized wall heat loss or wall convective transfer factor as tabulated against axial location, SSS (JS). Multiplied by QL (normalizing parameter) after reading.
QLS	HTL	Value looked up in Q (JS) table or radiation flux calculated in subroutine RDFLX.
QRAD	F1	Radiation heat loss per unit value.
RAT (JX)	F2	Maximum of PKP (JX) and PKR (JX). Basis of ordering reactions.
RB (JP,2) RC (JP,2) RD (JP,2) RE (JP,2) RF (JP,2)	F1	Curve fit constants for enthalpy, entropy and Cp of each species. See page 5-14. RB = F_1 + F_2, RC = F_3, RD = F_4, RE = F_5 and RF = F_6.

TABLE 1. Continued

Variable	Common	Description
RH (JS)	F4	Density at each station as output, predictor value.
RHS (JE2)	F1	Right hand side of equations to be solved in FLAME. After inversion these become solution.
RML (JX, JS)	F4	Ratio of forwar to reverse rate of each reaction at each station as output.
RMU (JE, JX)	F2	Stoichiometric coefficient of each reactant species in each reaction.
RUU (JS)	EPRP	Generated in EPROP as $1/\bar{\mu}_1$, then modified in ACEF to include other axial convection factors.
SB (JP)	F1	Entropy/R of each species at pressure (not standard state). Later modified to be log K_p of formation.
SS (JS)	F4	Axial distance as calculated and output. Also used to interpolate input data from prior solution, in which case SS (JS) correspond to normalized axial distance parameter.
SSS (JS)	HTL	Table of axial distances against which Q (JS) are tabulated.
T	F1	Temperature.
TC (JP)	F1	-HI (JP)/RT = -d log K_p/d log T.
TCOE	EPRP	Temperature coefficient on axial energy flux in flame energy equation.
TERM2	F1	Composite term used in wall flux calculation developed in ACEF, and invariant in FLAME.
TERV2	F1	Composite term used in volumetric heat loss calculation developed in ACEF, and invariant in FLAME.
THMU (JE1,JX)	F2	Third body efficiency of each species in each kinetic reaction. First subscript at IS + 1 yield efficiencies for general third body.

TABLE 1. Concluded

Variable	Common	Description
TITLE	F4	80 character title of problem set.
TL (JS)	F3	Temperature array as output for each station (predictor values).
TTT	F1	Exponent on T for wall flux term in mass and energy balances.
TTV	F1	Exponent on T for volumetric heat loss term in energy balance.
TU (JP,2)	F1	Temperature at which switch is made from low temperature to high temperature thermodynamic data curve fits (see page 5-14).
TW	F1	Wall temperature.
TWL (JS)	F3	Not used.
UNIT (JQ,JQ)	F1	Set of vectors used to rearrange FLAME coefficient matrix during introduction of kinetic equations. After inversion of matrix, application of vectors in reverse order restores inverse of non-rearranged matrix. Also used as on-diagonal matrix in corrector solution.
VNU (JP,JE)	F1	Stoichiometric coefficients for equilibrium reactions.
WM (JP)	LIN	Molecular weight of each species as input.
WML (JS)	F4	Molecular weight array as output for each station (predictor values).
XALPE (JP)	WANTS	ALPE (JP) as read.
XALPF (JP)	WANTS	ALPF (JP) as read.
XX (JX)	F2	Saved values of FKF (JX) prior to pressure and third body modifications.

TABLE 2. LOCAL VARIABLES

Variable	Definition
ACEF	Main Routine
ALD	Locally defined and used.
ALZISP	ALPHZ (IS + 1).
API	Input value for APR. If nonzero, APR set equal to API.
APR	Parameter defined by Eq. 36, or as described in card set 3.
APRR	Value of APR read from restart cards.
BLANK	Holerith field of blanks.
BPR	BP value read from restart cards.
CPTW	Value of C_p at wall conditions as used in wall heat flux calculations.
CTKN (JX)	Contribution of each reaction to specific mass balance as output.
DA	Predicted correction in APR based on predictor logic.
DAR (JQ,JS)	In predictor logic, the set of vectors representing the coefficients on APR for each equation at each station.
DCL (JQ)	Coefficients on $\alpha_{i_{n-1}}$ terms.
DCR (JQ)	Coefficients on $\alpha_{i_{n+1}}$ terms.
DEN	Locally defined variable.
DIS	Axial distance used in look up of QLS in Q (JS) vs. SSS (JS) table.
DIST	Used to generate SS (JS) for plug flow reactor problems.
DLS (JS)	Nodal width of each station.
DMAX	Damping parameter for corrector step.

TABLE 2. Continued

Variable	Definition
DOTM	Assigned $\dot{m}$ for flame problems.
DS (JS)	Input axial step size. In flame problems DS = σ.
DTIL	$\hat{D}$ with definition implied by EQ. 8.
DUM, DUML, DUMMX, DUMR, DUMZ	Locally defined variables.
EM12	Equals $M_{n-1,n}$ in Eq. 35.
EM21	Equals $M_{n,n-1}$ in Eq. 35.
EM23	Equals $M_{n,n+1}$ in Eq. 35.
EM32	Equals $M_{n+1,n}$ in Eq. 35.
FACT	Locally defined variable.
FCN (JE)	Convective flux into nodal volumes.
FFF	Locally defined variable.
FIB	Locally defined variable.
HDN	Locally defined variable.
I	Locally defined index.
IALF	Input data flag, see page 5-2.
IAP	Input data flag, see page 5-2.
IARG	Subroutine argument indicating remaining seconds in run.
ICT	Input data flag, see page 5-2.
IEN	Locally defined index.
IFV	Input data flag, see page 5-3.
IH	Input data flag, see page 5-8.
IJ	Locally defined index.

TABLE 2. Continued

Variable	Definition
IKAP	Input data flag, see page 5-3.
IKN	Input data flag, see page 5-3.
INA	Input data flag, see page 5-2.
INPCH	Output data flag, nominally 1, set to 2 when IARG < 20 or converged or last iteration.
INS	Number of entries in Q (JS) vs. SSS (JS) table.
IQ	Locally defined flag to RERAY.
ISS	= IS + 2.
IS2	= IS + 2.
IS3	= IS + 3.
IT	Iteration count in ACEF.
ITAB	Absolute value of ICC.
ITC	Input data flag, see page 5-2.
IWSR	Well stirred reactor flag.
I2, J, JJ	Locally defined indexes.
JQI	Running index in local table look up.
JQS	Number of sectors in overlay set.
JQS2	2*JQS
K	Locally defined index.
KAP	Input data flag, see page 5-3.
KR77	Locally saved value of KR7.
K2	Locally defined index.
LL	Locally defined index.
LM1	Locally defined index.

TABLE 2. Continued

Variable	Definition
LST	Flag indicating status of NTRAN
M	Locally defined index.
MCTT (JX)	Locally defined indexes.
MDOT	Flag indicating a flame problem with assigned mass flowrate.
MM	Locally defined index.
MZ	Locally defined index.
NCTT	Locally defined index.
NFH	Input data flag, see page 5-4.
NIS	Number of species in initial guess dataset, see page 5-12.
NIT	Number of corrector step iterations,see page 5-2.
NITM	Locally defined index.
NL	Number of axial stations or well stirred reactor solutions plus one.
NN	Locally defined index.
NODRV	Diagnostic flag, inactive.
NRA (6)	Names of radiating species.
NS	Number of stations in initial guess data set, see page 5-12.
NVL	= 0
NZ	Locally defined index.
PINT	Saved initial value of PM.
PMS	Saved converged value of PM.
PPB (JS)	Table of pressures for assigned T and P problems.

TABLE 2. Continued

Variable	Definition
QL	Input nomalizing flux (QL) or transfer coefficient (Cj). See page 5-7 or 5-8 respectively.
R	= 82.057, perfect gas constant
RATIO	Locally defined interpolation variable.
RTDD	Locally defined variable related to time.
RTDS	Composite parameter for distance calculation from transformed variables ($=ds/d\sigma$).
SADB, SADB2	Composite "parameter" for time, distance and flame speed.
SCALE	Damping parameter for corrector step.
SCMN	Schmidt Number raised to m-n power as used in wall flux calculations.
SM	Locally defined summation of DS(L).
SMP	Locally defined summation variable.
SMRT (JE)	Kinetic production term in nodal volume as output.
SMTT (JE)	Diffusive flux into a nodal volume as output.
SN	Locally defined summation of SS(L)
SNM	Locally defined interpolation variable.
SPB	P/BP
SPD	Flame speed as locally calculated and output.
STEP	Factor used to reduce axial or time step size if FLAME does not converge.
SUM	Locally defined summation variable.

TABLE 2. Continued

Variable	Definition
TCON	Right hand side of constraint equation for evaluation APR in corrector step.
TERM1, TERV1	The station independent parameters used in calculating the wall fluxes and volumetric heat loss, respectively.
TFLAME	Input assigned flame holder temperature (see page 5-6).
TIME	Summation of APR*AP(L) -- a time parameter equated to DTT(L) for KR6 = 1.
TINT	Initial temperature.
TKAP	Concentration or temperature constraint value input. See page 5-6.
TSQ	TW*TW
TTDS	Composite parameter for time calculation in transformed coordinates (=$dt/d\sigma$)
TTS	Saved value of temperature from most recent converged FLAME solution.
TVECA	Coefficient on temperature when temperature used as grid constraint variable.
VB, VC, VD	Locally defined variables used in thermodynamic property calculations.
VMU1, VMU2	Variables μ_1, and μ_2 as defined by Eq. 5 for bulk gas mixture.
VMU12, VMU21, VMU23, VMU32	Variables μ_{ij} as defined by EQ. 35 where indices n-1, n and n+1 are indicated by 1, 2 and 3, respectively.
V1	Locally defined variable.
WMU1, WMU3	The variables μ_1, and μ_3 as defined by equations 5 and 25, respectively, as evaluated at the wall for the wall flux terms.

TABLE 2. Continued

Variable	Definition
FLAME	Subroutine
ALPM	Equals log of PM.
ALT	Equals log of T.
BE	Exponent on PM for kinetic terms for various mass balance options.
BIG (JE)	Largest positive contribution to each mass balance. After kinetics package becomes largest absolute contribution.
BIGIE	Locally defined variable.
BIGN (JE)	Largest negative contribution to each mass balance.
BIGPN, BIGPP	Locally defined variable
BUMP	Factor to temporarily kick solution toward equilibrium for convergence purposes.
BUST	Value assigned to BUMP
CPTB	Local value of $\widehat{C}_p$ as used in wall convective fluxes.
CPTW	Wall value of $\widehat{C}_p$ as used in wall convective fluxes.
DAMP	Vactor used to scale down all corrections developed for each iteration.
DNE	Number of reactants in a kinetic reaction.
DNT	Check sum to establish presence of third body reactant.
DOM	Log of mole fraction of a species.
DUM, DUMB, DUM1, DUM2, DUM3	Locally defined variable.
EMAX	Maximum correction in species partial pressure on a given iteration

TABLE 2. Continued

Variable	Definition
EMXP	EMAX from prior iteration.
ESUM	Locally defined variable.
FACT	Locally defined factor used in restructuring mass balance equation toward equilibrium form.
G	Free energy of a species.
GN, GP	Locally defined to avoid divide by zero.
HTB	Local value of $\hat{h}$ as used in wall convective fluxes.
I	Locally defined index.
ICB	Count of iterations with BUMP activated.
ICT	Number of extra iterations after convergence test satisfied.
II, IK, IP	Locally defined indices.
ISS	Equals IS+2.
ITMX	Maximum number of iterations allowed.
I1, I2	Lower and upper limit of equation indices to which a given kinetic reaction will be added.
J, JJ, J1, K, K1	Locally defined indices.
LL (JE)	For the Kth mass balance, LL(K) = IK if the kinetic reaction of rank IK (IK - 1 for fastest reaction) is isolated into that mass balance. Otherwise LL(K) = 0.
MM	Locally defined index.
MX	Limit on DO loop for bubble ordering scheme.
NUL	= 0.
PLIM	Maximum allowed change in log partial pressures.
R	Perfect gas constant, 1.9865.

TABLE 2. Continued

Variable	Definition
RATIO	Local interpolation parameter.
RRT	Equals 1/RT.
RT	Equals R*temperature.
SCMN	Schmidt Number raised to m-n power (see Eq. 13).
SUMD, SUMH, SUMHT, SUMK, SUMR	Locally defined summation variables.
TCPMT	Locally defined product variable.
TERM	Locally defined wall flux variable.
TERM 3	Locally dfined wall flux variable.
TEST	Locally defined test variable.
TSQ	T*T
TST	Locally defined small number test variable.
TST1, TST2	Locally defined test variables.
VA, VB, VC, VD, VE, VF	Locally defined variables.
VLK	Log of k_f (see Eq. 12).
VMU1	Value of μ_1
VMU2	Value of μ_2
VQ	Volumetric heat loss rate.
V1, V2	Locally defined variables
WATE	Locally defined weighing parameter.
WJ	Wall species flux term.
WMU1	Value of μ_1, used in wall fluxes
WMU3	Value of μ_3 used in wall fluxes
WQ	Wall heat flux term.

TABLE 2. Continued

Variable	Definition
READIN	Subroutine
I	Local index.
IEND	Flag indicating end of input species set.
ISPECI	Species name.
J	Local index.
JMAX	Maximum number of species limit. Equal to JP.
XBP	Diffusion factor. Equal to BPA(J).
XE, XF	Species concentrations, first guess and initial respectively. Equal to ALPE(J) and ALPF(J) respectively.
OBTAIN	Subroutine
I	Local index.
IDUM	Used in skipping over nonrelevant thermochemical (T.C.) data files.
IEND	Flag which defines end of the data file.
IEOF	flag indicating end of data file.
IHDG	Used to skip over T.C. file title.
ITEST1, ITEST2	Used in matching species name to T.C. data file names.
J	Local index.
J1, J2	Index for equivalenced species names.
LNGTH	Length of T.C. data files
MATCH	Flag indicating match of species names and T.C. file names.
NLNGTH	Length of T.C. data files
OK	Flag indicating T.C. data for unknown species has been requested.

TABLE 2. Continued

Variable	Definition
GETDAT	Subroutine
K	Local index.
RA	Heat of formation in curve fit data.
ZZ	Used to print temperature bounds of curve fit T.C. data.
KINKIN	Subroutine
FX	Exponent on power of 10 part of coefficient a in equation 12.
I	Local index.
IFLAG	Stops program if there is a problem with kinetic data.
II	Local index used in equivalencing.
ISW	Flag on whether a species name in a reaction can be matched with the species input names.
JJ, J1, J2, K	Local index used in equivalencing.
KIN	Input unit designation.
KNY	Flag indicating equivalenced species name.
KOUT	Output unit designation.
L, M	Local index.
MLET	Third body flag name.
NA, NB	Species name in reactions.
NT, NTB	Name of individual third body.
PSUM, RSUM	Used in reaction balance check.
TB	Third body efficiency.

TABLE 2. Continued

Variable	Definition
EPROP	Subroutine
CPGS, CPG1	Gas specific heat at first station and at previous station respectively.
CPTILS, CPTIL1	Weighted gas specific heat at first station and at previous station respectively.
EM12, EM21	Defined the same as in ACEF.
I, J	LOCAL index.
KRS	Save KR in KRS.
KR6S	Save KR6 in KR6S.
L	Local index.
NL	Last station.
RLB	Average of upstream and downstream Lewis number parameter.
RL1, RL2, RL1S	Reciprocal of Lewis number parameter at upstream and downstream stations and first station respectively.
U11, U12, U21, U22 U11S, U21S	Variable μ_1 as defined in Equation 5 for various stations.
VMU1, VMU12, VMU21, MVU3, VMU6	Variable μ_2 as defined in Equation 5 for various stations.
RDFLX	Subroutine
DKPDT	Derivative of absorption coefficient with respect to temperature.
FAC	Local variable as defined.
I1, I2, I3, J	Local index.
PKCO, $PKCO_2$, PKH_2O	Planck mean absorption coefficient for CO, CO_2 and H_2 respectively.

TABLE 2. Concluded

Variable	Definition
PPI1, PPI2, PPI3	Partial pressure of CO_2, H_2O and CO respectively.
RATIO	Interpolation ratio.
SIGMA	Stefan-Boltzmann constant.
SUMKP	Composite absorption coefficient.
TEMP	Temperature.
T1, T2, T3	Derivative of absorption coefficient with temperature.
XKPCO, $XKPCO_2$, $XKPH_2O$	Planck mean absorption coefficients in table form

SECTION 10

PROGRAM AND SUBROUTINES

Brief descriptions of the PROF main program and subroutines are given in this section. The code consists of the main program, ACEF, and eight subroutines.

10.1 ACEF Main Program

The main program, ACEF, has a number of functions and serves as the driver for the chemistry solver routine.

ACEF initializes some constants and reads a variety of input parameters. Integral and nonintegral parameters, grid spacings and heat loss data are read by ACEF. Subroutines READIN, OBTAIN and KINKIN are called by ACEF to read in initial species concentration, thermochemical and kinetic reaction data respectively. If needed, punched card first guess data is read by ACEF. Following this operation, the main program loop on grid solution iterations is entered. The EPROP subroutine is then called to calculate energy and species equation parameters at each grid point. These parameters are held fixed during each iteration cycle. In this loop, space or time step quantities and diffusion terms are constructed. The FLAME subroutine is then called to calculate the change in concentrations due to chemical kinetic reactions. Following this, output quantities are set up and the corrector step partial derivative matrix is constructed. The RERAY subroutine is then called to invert the corrector step matrix. Predictor/corrector step information is printed out and, for the last iteration or a converged solution, summary information is printed.

10.2 READIN Subroutine

This subroutine reads the species names, initial and final species concentrations and diffusion factors. If called for, this subroutine also equivalences species names so that names other than those on the thermochemical data file can be used on the initial concentration or kinetic reaction inputs.

10.3 OBTAIN Subroutine

This subroutine scans either the tabular or curve fit thermochemical data file for the species of interest. Once the proper species thermochemical data file is found, subroutine GETDAT is called to extract and store the data.

10.4 GETDAT Subroutine

This subroutine extracts tabular or curve fit thermochemical data from input/output unit 12 or 11 respectively and stores the data for use during a calculation.

10.5 KINKIN Subroutine

This subroutine reads in the kinetic reactions and their associated rates. It then developes the stoichiometric coefficients for the reactions and checks to see if the reactions balance. The stoichiometric coefficients are applied in the FLAME subroutine.

10.6 EPROP Subroutine

This subroutine develops the parameters which remain effectively constant in the energy and species equations during a predictor/corrector step iteration. The FLAME subroutine is called by EPROP to determine thermodynamic properties for a fixed composition and enthalpy. These properties are then used to generate composite parameters which are held fixed during the predictor/corrector step iteration.

10.7 FLAME Subroutine

This is the program's key subroutine which solves the species and energy equations including the effects of chemical kinetics. The routine begins by setting up the individual species thermochemical properties. If needed, the radiation heat loss subroutine, RDFLX, is then called to determine the gas mixture absorption coefficient. This coefficient is used in establishing radiative heat loss from the flame gases. Utilizing current solution estimates, errors and their derivatives with respect to the variables are formed for the enthalpy, total pressure and species mass balance equations. At this point, these equations include the effects of wall heat loss but do not include the effects of chemical kinetics. Chemical kinetic reaction contributions to the equations are constructed and ordered from fast to slow. These contributions are then factored into the equations making necessary equation rearrangements to introduce the dominant reactions into only a single mass balance equation. The resulting equation errors are then checked for convergence. If convergence is not achieved the matrix of error derivatives is inverted and multiplied by the errors to obtain the corrections to the variables needed to drive the equation errors to zero. If the corrections exceed a certain multiple of the variables, all of the corrections are uniformly damped so as not to overcorrect the variables. Corrections are then made and the solution procedure cycles to the top of the subroutine to repeat the above process until either a converged solution is found or the allowed number of iterations is exceeded.

10.8 RDFLX Subroutine

This subroutine uses correlations of Planck mean absorption coefficient data for H_2O, CO_2 and CO to develop the gas mixture absorption coefficient. This coefficient is used in the radiative heat loss model applied in the FLAME subroutine.

10.9 RERAY Subroutine

This subroutine is a generalized matrix inversion routine which either gives a set of solution vectors or the solution vectors plus the full matrix inversion.

SECTION 11

PROGRAM SOURCE DECK LISTING AND SYSTEM REQUIREMENTS

Listings of the PROF code main and subroutine Fortran V source decks are presented in this section. Also, sample problem run times and system requirements are presented below.

Sample Problem Run Time

Computation time depends, of course, on the problem being computed. The times associated with each sample problem are given below.

Sample Problem	Time (sec)	
7.1	45	per iteration (roughly six iterations are need for convergence)
7.2	45	
7.3	60	
7.4	2	per individual solution
7.5	50	

Tape Requirements

Internal program assignments are as follows:

Tape Unit 5: Read
Tape Unit 6: Write
Tape Unit 7: Punch
Tape Unit 10: Unit number of NTRAN
Tape Unit 11: Curve fit thermochemical data
Tape Unit 12: Tabular thermochemical data

System Specifics

The specific UNIVAC 1108 exec 8 items used by the program are:

1. TLEFT (IARG)

   TLEFT returns the number of system seconds (as IARG) left before a maximum time abort will occur.

2. NTRAN (10, sequence of operation)

   NTRAN is used for writing and reading binary information, contained in the ARHM array, onto a drum. This operation of writing and reading onto a drum reduces the processor storage requirement which would be needed for the block tri-diagonal matrix solution procedure.

NTRAN roughly, corresponds to BUFFERIN and BUFFEROUT which are present on Control Data Corporation systems.

Storage Requirements

At least 15355 words decimal storage are needed for instruction and 31978 words decimal storage are needed for data.

ACEF - MAIN PROGRAM

```
      PARAMETER JP=29,JE=28,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
     *+2,JSM=JS-1,JQQ=JQ*JQ
C     JX=NO. OF REACTIONS
C     JP=NO. OF SPECIES
C     JS=NO. OF STATIONS
C     JE=NO. OF ELEMENTS
      DIMENSION NRA(6),PPR(JS),DCL(JQ),DCR(JQ),SMTT(JE),DAA(JE2,1),DLS(J
     *S)
      DIMENSION TVEC(JQ),DAR(JQ,JS),TINPT(20),TVECR(JQ)
      DIMENSION  DS(JS),TTR(JS),SMRT(JE),FCM(JE)
      COMMON/EPRP/RUU(JS),RMU(JS),CHI(JS),ALA(JQ,JS)
     *,CPTIL,HTCOE,TCOE
      COMMON/F4/TITLE(20),RML(JX,JS),PML(JX,JS),AX(JS),WML(JS),RH(J
     *S),HH(JS),SS(JS),DTT(JS)
      DIMENSION  CTKN(JX),MCTT(JX)
      COMMON/F3/ALPF(JQ),ALPE(JQ),ALPHZ(JQ),FLUX(JQ),PPI(JP),FPS(JP),
     *   ALB(JQ,JS),TL(JS),TWL(JS),AP(JS),AA(JE2,JE2),DUD(JQ),DUMB(JQ),
     *   ARHM(JQ,JQ),RPA(JQ),CKINI(JQ)
      COMMON/F1/RHS(JE2),A(JE2,JE2),E(JP),ALPHI(JQ),UNIT(JQ,JQ),
     *   VNU(JP,JE),RB(JP,2),RC(JP,2),RD(JP,2),RE(JP,2),RF(JP,2),
     *   TU(JP,2),PP(JP),PLP(JP),HI(JP),SB(JP),PPTC(JP),HOS(JP),
     *   TC(JP),CPF(JP),NAMA(JP),NAMB(JP),CPG,TW,HRC,PM,T,P,KK,KR6,KR7,
     *   N,IS,ISP,NEQ,MT,CKIN(JQ),H,PLN,ITER,ICON,IR,L,ICC,NFHS
     *,NRS(3),DQRDT,DQRDP(3),RP,PMW,FT,PW(JP)
     $   ,TERM2,TERV2,QRAD,TTV,PPV,TTT,PPP,FW(JP),CPWI(JP),ALFW(JE),CHIW
     $,  HTW,EXM,EXN,IH
      COMMON/F2/ THMU(JE1,JX),PPX(JX),RMU(JE,JX),PMU(JE,JX),PRMU(JE,JX),
     *   PKP(JX),PKR(JX),PMR(JX),XX(JX),DKPT(JX),FKF(JX),AFF(JX),
     *   EXK(JX),EAK(JX),RAT(JX)
     *  ,MP(JX),MA(JX)
      COMMON   /WANTS/   IWANT(3,JP),   NWANT,         XALPF(JP),
     $                   XALPE(JP)
      COMMON /LIN/ CPT(JP,50), HT(JP,50), GT(JP,50), HRF(JP), WM(JP)
     *,KNY,IQV(16,4),ALDEN(JP)
      COMMON/HTL/SSS(JS),Q(JS),QLS,EGYDS
      EQUIVALENCE (A,DAA)
      DATA  (NRA(J),J=1,6)/4HCO2 ,4HH2O ,4HCO  ,4HENTL ,4HTEMP,4HHTIL /
      DATA BLANK/4H    /
  205 FORMAT(8E10.5)
  206 FORMAT(2X,2I4,9F12.7/(1X,10E12.7)/(2X,10E12.7))
   50 FORMAT(6H FLUX ,10E10.4/(1X,10E10.4))
  405 FORMAT(24F3.0)
  410 FORMAT(1X,  24F4.1)
      NUL=0
      NIS=0
      ICC=0
C             NUMBER OF SECTORS IN OVERLAY SET (28WORDS PER SECTOR)     RMK10057
      JQS=(JQQ+27)/28
      JQS2=JQS+JQS
      R=82.057
   53 READ(5,210) TITLE
  210 FORMAT(20A4)
      WRITE(6,214)
  214 FORMAT(1H1,25X,51HPREMIXED ONE DIMENSIONAL FLAME CODE SOLUTION (PR
      *OF),///24X,52HPROGRAM DOCUMENTED IN THE "PROF CODE USER'S MANUAL",
      */ 26X,       43HAEROTHERM/ACUREX CORP FINAL REPORT 78-277        ,/
      *  34X,           20HPHONE 415/964-3200                 ,///)
       WRITE(6,211) TITLE
   211 FORMAT( 5X,20A4//)
       EXM=1.0
       EXN=1.0
       IWSR=0
       NODRV=0
       READ(5,208)IS,KR6,N,NL,NIT,INA,IALF,IAP,ITC,IFV,IKN,IKAP,KAP,KR7,
      *NFH,MDOT
       IF(ITC.NE.0) ICC=ITC
       IF(ICC.EQ.0) STOP ITC
       KR77=KR7
       IF(IKN.GE.0) GO TO 50001
       IKN=-IKN
       KR=1
 50001 CONTINUE
       ITAB=IABS(ICC)
       IF(IS.EQ.0)GO TO 301                                            RMK10107
       WRITE(6,209)IS,KR6,N,NL,NIT,INA,IALF,IAP,ITC,IFV,IKN,IKAP,KAP,KR7,
      *NFH,MDOT                                                        RMK10107
       IF(KR6.LE.-2) NODRV=1
       IF(KR6.LE.-2) KR6=-KR6
       ISP = IS + 1                                                    RMK10057
       IS2 = IS + 2                                                    RMK10057
       IS3 = IS + 3                                                    RMK10057
       NEQ=IS                                                          RMK10107
       IF(ITAB.NE.1.OR.NFH.NE.0) NEQ=ISP
       IF(KR6.EQ.3 ) NEQ=IS+3
       IF(KR6.EQ.3) KR6=2
       IF(KR6.EQ.-1) IWSR=1
       IF(KR6.EQ.-1) KR6=0
       IH=0
C              READ NON-INTEGER                                        RMK10057
       READ (5,205) API,BP,P,T,TKAP,TFLAME
       WRITE(6,541) API,BP,P,T,TKAP,TFLAME
       BP=AMAX1(BP,1.E-20)
       DTIL=0.172E-4/P
   541 FORMAT(1H0,33X,26H* NONINTEGRAL PARAMETERS *///6X,13HAPR=DEL/MDOT=
      *,E10.5,3X,19HBP=DPAR/(DEL*MDOT)=,E10.5,4X,2HP=,F8.3,5H(ATM),
      *7H   TI=   ,F7.1,4H(K)    //12X,5HTKAP=    ,F10.5,
      *3X,7HTFLAME=,F7.1,3H(K)///)
C      FOR SUBSEQUENT RUNS STORED APR IS USED WHEN API LT 0
       IF (API .LE. 0.) GO TO 32                                       RMK10057
       APR = API                                                       RMK10057
       IF (MDOT .NE. 1) GO TO 32                                       RMK10057
       DOTM = APR                                                      RMK10057
       APR = .172E-4 / (P*BP*DOTM*DOTM)                                RMK10057
       WRITE (6,70) DOTM                                               RMK10057
    70 FORMAT(10X,15HMASS FLOWRATE=  ,E10.5)
    32 IF(IAP.EQ.0) GO TO 61                                           RMK10057
C              READ GRID PARAMETERS                                    RMK10057
       READ(5,44) (AP(I),I=1,NL)                                       RMK10057
       READ(5,44)(DS(I),I=1,NL)                                        RMK10057
       WRITE(6,36) NL                                                  RMK10057
       WRITE(6,41)(AP(I),I=1,NL)                                       RMK10057
      TERV1=1.0
      PPV=1.0
      TTV=0.
      IF(KR6.NE.2) GO TO 409
      DO 408 I=1,NL
  408 AP(I)=AP(I)*AP(I)
      TERV1=1./R
      PPV=2.
      TTV=0.659
  409 WRITE(6,136) NL
  136 FORMAT(1H0,10X,14H SIGMA(N),N=1,,I3/)
      WRITE(6,41)(DS(I),I=1,NL)                                         RMK10057
   36 FORMAT(1H0 ,34X,19H* GRID PARAMETERS *// 10X,14H A(N)**2 ,N=1,,I3/
     *)
   41 FORMAT(10X,10E10.4/15X,10E10.4/20X,10E10.4/25X,10E10.4//)
   61 IF (KR6 .NE. 1) GO TO 217                                         RMK10057
C     READ T AND P ASSIGNMENT FOR EACH GRID POINT
      READ(5,412) (TTB(I),I=1,NL)
      READ(5,412) (PPB(I),I=1,NL)                                       RMK10107
      WRITE(6,415)
  415 FORMAT(1H0,30X,33H* ASSIGNED T AND P DISTRIBUTION * //)
      WRITE (6,413) (TTB(I), I=1,NL)                                    RMK10057
      WRITE (6,414) (PPB(I),I=1,NL)                                     RMK10107
  412 FORMAT(8E10.5)
  413 FORMAT(5X,29HTEMPERATURE DISTRIBUTION (K)      /
     $5X,8E12.5/10X,8E12.5/15X,8E12.5/20X,8E12.5/)
  414 FORMAT(1H0,5X,26HPRESSURE DISTRIBUTION(ATM)  /5X,8E12.5
     $/10X,8E12.5/15X,8E12.5/20X,8E12.5/ )
  217 IF(ITAB.EQ.1.OR.ITAB.EQ.3) GO TO 5000
C     READ ENERGY LOSSES OR C-SUB-J AS A FUNCTION OF DISTANCE
      WRITE(6,416)
  416 FORMAT(1H0,36X,18H* HEAT LOSS DATA *  //)
 5009 READ(5,5002) INS,QL
      WRITE(6,5001) INS,QL
      IF(INS.EQ.1)  GO TO 5010
      READ(5,412) (SSS(J),J=1,INS)
      READ (5,412) (Q(J),J=1,INS)
      WRITE(6,5005) INS
      WRITE(6,5008)  INS
      DO 5006 J=1,INS
 5006 Q(J)=Q(J)*QL
      WRITE (6,501) (Q(J),J=1,INS)
      WRITE(6,501)  (SSS(J),J=1,INS)
 5008 FORMAT(15X,13HSS(N),N=1,INS)
 5010 IF (ITAB.LT.4) GO TO 5000
C              READ WALL TEMPERATURE AND RELATIVE MOLE CONCENTRATIONS   RMK10057
      READ(5,5002) IH,TW,EXM,EXN
 5007 FORMAT(12X,19HWALL HEAT LOSS DATA    )
      WRITE (6,5003) IH, TW                                             RMK10057
      WRITE (6,5012) EXM,EXN
      TTT=0.3295*EXM
      PPP=1.+EXM
      TERM1=4.*(TW**0.3295*DTIL/R)**EXM
      IF(KR6.NE.2) GO TO 5011
      TERM1=TERM1/R
      TTT=TTT+0.659
      PPP=PPP+1.0
 5011 IF(IH.LE.1) GO TO 5000
      READ(5,44) (PW(J),J=1,IS)
      WRITE(6,5510)                                                      RMK10107
 5510 FORMAT(10X,28HWALL SPECIES CONCENTRATIONS //)
      WRITE (6,5004) (PW(J),J=1,IS)                                      RMK10107
 5004 FORMAT(10X,8E10.5/25X,8E10.5/40X,6E10.5)
 5002 FORMAT(I4,6X,5E10.5)
 5003 FORMAT(15X,15HREACTIVITY PAR=,I2,4X,10HWALL TEMP=,E10.5//)
 5012 FORMAT(15X,19HREYNOLDS FXPONENT =E10.5, 5X,18HSCHMIDT EXPONENT =
     $E10.5//)
 5001 FORMAT(10X,16HNO. OF STATIONS=,I4,8X, 4HQLS=,E10.5 //)
 5005 FORMAT(15X,13HQ(N)/QLS,N=1,  ,I3)
  208 FORMAT(16I3)
  209 FORMAT(33X,23H* INTEGRAL PARAMETERS *,//T4, 6HCOLUMN,T54,6HCOLUMN,
     */T6,33H 3  NO. SPECIES CONSERVATION EQS.,T40,I3,T56,31H 6  PROBLEM
     * TYPE AND ENERGY EQ.,T90,I3,//
     *,T6,18H 9  NO. OF SPECIES, T40,I3,T56,
     *T56,23H12  NO. AXIAL GRID PTS.,T90,I3,//,T6,32H15  NO. GRID SOLUTI
     *ON ITERATTONS,T40,I3,T56,30H18  SOLUTION CYCLE CONTROL NO.,T90,I3
     *//T6,30H21  READ INITIAL MOLE FRACTION,T40,I3,T56,31H24  READ NONI
     *NTEGRAL PARAMETERS,T90,I3,//,T6,33H27  THERMO DATA & HEAT LOSS MOD
     *EL ,T40,I3,T56,21H30  CONSTRAINT SWITCH,T90,I3,//,T6,21H33  READ K
     *INETIC DATA,T40,I3,T56,34H36  CONSTRAINT APPLIED TO VARIABLE,T90,
     *I3,//,T6,34H39  CONSTRAINT APPLIED TO GRID PT.,T40,I3,T56,22H42  O
     *UTPUT CONTROL NO.,T90,I3,//,T6,34H45  FLAMEHOLDER TEMP ASSIGN SWIT
     *CH,T40,I3,T56,30H48  INPUT MASS FLOWRATE SWITCH,T90,I3,//)
 5000 DMAX=.001
      IF(IALF.EQ.0)GO TO 16
      ISP=IS+1
C
C              READ SPECIE NAMES, INITIAL RELATIVE MOLES, GUESSED FINAL  RMK10057
C              RELATIVE MOLES, DIFFUSION FACTORS, AND NAMES EQUIVALENCE  RMK10057
C              TABLE                                                     RMK10057
      CALL  READIN
      DO 14 I=1,N
   14 BPA(I)=BPA(I)*BP
C
      IF (NWANT .EQ. IS) GO TO 16
      WRITE (6,20011) NWANT, IS
20011     FORMAT (39H0*** PROGRAM STOPPED IN MAIN ROUTINE --, I5,
     $            27H SPECIES REQUESTED BUT IS =, I5, 4H ***
     $)
         GO TO 301
C
   16 IF(ITC .EQ. 0)  GO TO 13
C              OPTAIN SPECIES MOLECULAR WEIGHT AND THERMOCHEMICAL        RMK10057
C              DATA FROM FILES                                           RMK10057
      CALL  OBTAIN
C
C              FOLLOWING CORRECT FOR N = IS ONLY                         RMK10057
      DO 2 I = 1, N
      DO 3 J = 1, IS
      VNU(I, J) = 0.0
    3 IF(I .EQ. J)  VNU(I, J) = 1.0
    2 CONTINUE
      IF(IS.EQ.N) GO TO 39
      DO 38 I=ISP,N
   38 PPI(I)=1.E-10
   39 CONTINUE
C
   13 IF(IH.EQ.0) GO TO 15
      IF(ITC.GT.0) GO TO 372
      VB=TW-3000.
      VC=(TW+3000.)/2.
      VD=TW*3000.
      TSQ=TW*TW
      DO 371 I=1,N
      J=2
      IF(TW.LT.TU(I,1))J=1
      CPWI(I)=RC(I,J)+T*RD(I,J)+RE(I,J)/TSQ
  371 HI(I)=RB(I,J)+VB*(RC(I,J)+RD(I,J)*VC+RE(I,J)/VD)
      GO TO 374
  372 J=TW/100.
      J=MAX0(1,J)
      J=MIN0(J,49)
      RATIO=TW*0.01-FLOAT(J)
      DO 373 I=1,N
      CPWI(I)=CPT(I,J)+RATIO*(CPT(I,J+1)-CPT(I,J))
  373 HI(I)=HRF(I)+HT(I,J)+RATIO*(HT(I,J+1)-HT(I,J))
  374 DO 375 I=1,N
  375 FW(I)=(BP/BPA(I))**EXN
      IF(IH.LE.1) GO TO 15
C     NORMALIZE WALL CONCENTRATIONS TO PARTIAL PRESSURES
      DUM=0.
      PMW=0.
      DO 230 I=1,IS
  230 DUM=DUM+PW(I)
      DUM=P/DUM
      DO 37 I=1,IS
      PW(I)=PW(I)*DUM
   37 PMW=PMW+WM(I)*PW(I)
      VMU2=0.
      VMU1=0.
      WMU1=0.
      WMU3=0.
      HTW=0.
      CPTW=0.
      DO 376 I=1,N
      VMU1=VMU1+PW(I)/BPA(I)
      WMU1=WMU1+PW(I)*FW(I)
      VMU2=VMU2+PW(I)*BPA(I)*WM(I)
      V1=PW(I)/FW(I)
      HTW=HTW+V1*HI(I)
      CPTW=CPTW+V1*CPWI(I)
      WMU3=WMU3+V1
  376 ALFW(I)=PW(I)/PMW
      HTW=HTW/PMW
      CPTW=CPTW/PMW
      WMU1=WMU1/P
      VMU1=VMU1/P*BP
      VMU2=VMU2/(P*BP)
      CHIW=1.9865*.29*WMU3/PMW
      SCMN=(VMU2*P/(PMW*1.344*VMU1))**(EXM-EXN)
      TERM1=TERM1*SCMN*PMW**(EXM/2.)/WMU1
      PPP=PPP-EXM/2.                                                    RMK10057
C              READ KINETIC DATA
   15 IF(IKN.GT.0) CALL KININ
      IF(IKN.GT.0) KR=5                                                 RMK10057
C              IDENTIFY INDECIES ON RADIATION SPECIES                   RMK10057
C              CO2, H2O, CO
      DO 3402 I=1,3
 3402 NRS(I) = 0
      DO 3401 J=1,N
      DO 3401 I=1,3
 3401 IF(NRA(I).EQ.NAMA(J)) NRS(I)=J
 3404 FORMAT(5X, 3I5)                                                   RMK10057
C              NORMALIZE ALPF AND ALPE
      WML(1)=0.                                                         RMK10057
      DUM = 0.                                                          RMK10057
      SMP = 0.                                                          RMK10057
      DO 3400 I=1,IS                                                    RMK10057
         SMP = SMP + ALPF(I)
      WML(1)=WML(1)+ALPF(I)*WM(I)                                       RMK10057
         DUM = DUM + ALPE(I)*WM(I)                                      RMK10057
 3400 CONTINUE                                                          RMK10057
      DO 3500 I=1,IS
      ALPF(I)=ALPF(I)/WML(1)                                            RMK10057
         ALPE(I) = ALPE(I) / DUM                                        RMK10057
 3500 CONTINUE                                                          RMK10057
      WML(1) = WML(1) / SMP                                             RMK10057
      DO 55 I=1,IS
      CKINI(I)=0.
      ALPHI(I)=ALPF(I)
      ALA(I,1)=ALPHI(I)
   55 ALB(I,1)=ALPHI(I)
      INPCH=1
      PM=P*WML(1)                                                       RMK10107
      IF(KR6.NE.1) GO TO 59                                             RMK10107
      T=TTB(1)                                                          RMK10107
      P=PPR(1)                                                          RMK10107
   59 CONTINUE
      PLN=ALOG(P)
      HTCOE=0.
      TCOE=0.
      ALA(IS+2,1)=T                                                     RMK10057
      TINT = T
      PINT=PM                                                           RMK10057
      TL(1) = T
      QLS=0.
C     ****CALL EPROP (1,1) ***** WHICH CALCULATES PROPS AT FIRST STATION RMK10057
      CALL EPROP (1, 1)
      DO 62  J=ISP,IS3
      ALPHZ(J)=0.
      ALA(J,1)=ALPHI(J)
   62 ALB(J,1)=ALPHI(J)
      HH(1)=ALA(ISP,1)
      IF (IALF .EQ. 0.OR.IALF.EQ.2) GO TO 60
      DEN=NL-1
      DO 10  I=1,IS
      DO10 L=2,NL
      FACT=L-1
      FACT=FACT/DEN
      IF(IWSR.EQ.1) FACT=1.
   10 ALA(I,L)=ALPE(I)*FACT+ALPF(I)*(1.-FACT)
   60 IF(MOD(INA/2,2).EQ.0) GO TO 42
C              READ DETAILED RESTART INFORMATION AND INTERPOLATE         RMK10057
C              IF NECESSARY                                              RMK10057
      WRITE(6,2140)
      READ(5,210) TINPT
      WRITE(6,210) TINPT
      READ(5,2080) NS,NIS,APRR,BPR
      IF(APRR.GT.0..AND.MDOT.EQ.0)  APR=APRR
      IF(BPR.GT.0.) BP=BPR
      IF(MDOT.EQ.1) APR=.172E-4/(P*BP*DOTM*DOTM)
      READ(5,48) (SS(L),L=1,NS)
      WRITE(6,2130) NS
 2130 FORMAT(1H0,10X,21HNORMALIZED  S(N),N=1,  I2//)
      WRITE(6,44) (SS(L),L=1,NS)
      READ(5,48) (ALB(ISP,L),L=2,NS)
      WRITE(6,2150) NS
 2150 FORMAT(1H0,10X,21HENTHALPY(CAL/GM),N=1,  I2//)
      WRITE(6,44)  (ALB(ISP,L),L=2,NS)
 2080 FORMAT (2I3,3E10.5)
      WRITE(6,2160) NIS,NS
 2160 FORMAT(1H0,10X, 16H(ALPHA(I,N),I=1,,I2, 5H,N=1,,I2,1H) //)
 2140 FORMAT(1H1,30X,24H* FIRST GUESS ALPHAS *  // )
      DO1043  I=1,NIS
      READ(5,48)(ALB(I,L),L=2,NS)
 1043 WRITE(6,44 ) (ALB(I,L),L=2,NS)
      IF(APRR.GT.0.) WRITE(6,2180) APRR,BPR
 2180 FORMAT(1H0,15X,5HAPRR=,E10.5,6X,4HBPR=,E10.5   )
      SN=0.
      SM=0.
      J=0
      DO2000 L=2,NL
      SM=SM+DS(L-1)
 2005 IF(SN.GE.SM) GO TO 2001
      IF(J.EQ.NS-1) GO TO 2002
      J=J+1
      SN=SN+SS(J)
      GO TO 2005
 2001 SNM=SN-SS(J)
      DUM=(SM-SNM)/SS(J)
      GO TO 2004
 2002 DUM=1.
 2004 ALA(ISP,L)=ALB(ISP,J+1)*DUM+ALB(ISP,J)*(1.-DUM)
      DO 2000  I=1,NIS
      IF(ALB(I,2).LT.0.) GO TO 2000
      ALA(I,L)=ALB(I,J+1)*DUM+ALB(I,J)*(1.-DUM)
 2000 CONTINUE
      WRITE(6,2200) NL
 2200 FORMAT(1H0,/4X,38HSCALED  H AND ALPHA FIRST GUESS VALUES   ///
     * 8X, 9HH(N),N=1,,I3//)
      WRITE(6,212) (ALA(ISP,L),L=1,NL)
      WRITE(6,2210) IS,NL
 2210 FORMAT(1H0, 8X,15HALPHA(I,N),I=1,,I2,5H,N=1,, I2/)
      DC 43 I=1,IS
   43 WRITE(6,212)   (ALA(I,L),L=1,NL)
```

```
  213 FORMAT(1H0,8X,23HALPHA VALUES INPUT L=1,I3/)
  212 FORMAT(10X,8(E10.5,2X)/15X,8(E10.5,2X)/20X,8(E10.5,2X)/25X,8(E10.5
     1,2X)/)
   48 FORMAT(10F8.4)
   44 FORMAT(8E10.4)                                                    RMK10057
   42 CONTINUE
      DO 421 I=1,IS
      ALA(I,2)=AMAX1(ALA(I,2),1.E-30)
      PLP(I)=ALOG(ALA(I,2)*PM)
  421 PPI(I)=PLP(I)
      IF(KR6.NE.2) NIT=1
C   --BEGIN MAJOR LOOP ON ITERATIONS
 1328 DO 45   IT=1,NIT
      IF(KR6.NE.2) GO TO 33
C   ********************************
C     CALL TO EPROP CALCULATES PROPERTIES FOR STATIONS 2 TO NL
      CALL EPROP (2,NL)
C   ********************************
      IF(NFH.EQ.1) TL(2)=TFLAME
      DO 31  L=2,NL
   31 RUU(L-1)=RUU(L-1)/DS(L-1)*BP
   33 DC 40 J=1,N
      PLP(J)=PPI(J)
   40 PPS(J)=PLP(J)
      T=TINT
      IF(IWSR.EQ.1) T=TFLAME
      PM=PINT
      TTS=T
      PMS=PM
      SADB=SQRT(APR*AP(1)/BP*DTIL)
      RTDS=RH(1)*TL(1)**1.659*SADB
      TTDS=RH(1)*APR*AP(1)*RTDS/SADB
      DIS=0.
      SN=0.
      SM=0.
      JQI=0
      H=HH(1)
      SS(1)=0.
      DTT(1)=0.
      IF(KR7.GE.2.AND.INPCH.EQ.1) WRITE(6,52) IS
   52 FORMAT(1H1,/30X,38H* CHEMISTRY SOLUTIONS AT GRID POINTS *//
     *           3X,4HITER,2X,1HL,4X,2HPM,11X,1HT,11X,10HPP(I),I=1,,I2)
      IF(INPCH.EQ.1) GO TO 3218
      DUM=SQRT(.172E-4/(APR*AP(1)*P*BP))
      DO 5200 I=1,IS
      SMRT(I)=0.
 5200 FCN(I)=       ALA(I,1)*DUM
      WRITE(6,3217)      IT
 3217 FORMAT(1H1,20X,54H* MOLE FLUXES AT GRID POINTS(MOLE/(CM2*S)) ITERA
     *TION   ,I2, 2H *//
     *20X,58HREACTION CREATION/DIFFUSION FLUX OUT/CONVECTIVE FLUX OUT
     *    ////)
      L=1
      DLS(1)=0.
      WRITE(6,3214) L,DLS(1)
      WRITE(6,3213)     (NAMA(J),NAMB(J),J=1,IS)
      WRITE(6,501) (SMRT(I),I=1,IS)
      WRITE(6,501) (SMRT(I),I=1,IS)
      WRITE(6,501) (FCN(I),I=1,IS)
 3218 CONTINUE
C    ********************************************
C    BEGIN MAJOR LOOP ON STATIONS
      DO 27  L=2,NL
      IF(NFH.NE.0.AND.L.EQ.2) T=TFLAME
      SS(L)=0.
      IF(KR6.EQ.2) GO TO 218
      IF(KR6.EQ.0.AND.IWSR.EQ.0) SS(L)=SS(L-1)+DS(L-1)                    RMK10107
      IF(KR6.NE.1) GO TO 218                                               RMK10107
      T=TTB(L)                                                             RMK10107
      P=PPB(L)
      DTT(L)=DTT(L-1)+APR*AP(L)
  218 CONTINUE
      QLS=0.
      SADB=SQRT(APR*AP(L) /BP*DTIL)
      IF(ITAB.EQ.1.OR.ITAB.EQ.3) GO TO 6001
 6016 QLS=QL
      IF(INS.EQ.1) GO TO 6001
      IF(KR6.EQ.2) GO TO 6006
      DIS=SS(L)
      GO TO 6003
C       CALCULATE DISTANCE FROM TRANSFORMED COORDINATE
 6006 CONTINUE
      DIS=DIS+(RTDS+RH(L)*TL(L)**1.659*SADB)*DS(L-1)*.5
C     LOOK UP HEAT LOSS PARAMETER AS FUNCTION OF DISTANCE
 6003 JQI=JQI+1
      IF(JQI.GE.INS) GO TO 6004
      IF(SSS(JQI).LT.DIS) GO TO 6003
      SNM=SSS(JQI)-SSS(JQI-1)
      SNM=(DIS-SSS(JQI-1))/SNM
      QLS=(Q(JQI)-Q(JQI-1))*SNM+Q(JQI-1)
      JQI=JQI-1
      GO TO 6001
 6004 QLS=Q(INS)
 6001 CONTINUE
      IF(KR7.GT.2)WRITE(6,6111)JQI,DIS,SS(L),QLS
 6111 FORMAT( 5X,6HQLOSS=,I4,3E10.5)
      CKINI(1)=APR*AP(L)*(DS(L)+DS(L-1))*.5
      TERV2=CKINI(1)
      IF(KR6.NE.2) TERM2=TERV2*QLS*(APR*AP(L))**(EXM-1.)
      LM1=L-1
      IF(IWSR.EQ.1) LM1=1
      DO 56 I=1,IS
      ALPHI(I)=ALB(I,LM1)
      ALDEN(I)=1.0
   56 CKINI(I)=CKINI(1)
      HDN=1.0
      ALPHI(ISP)=ALB(ISP,LM1)
      IF(KR6.NE.2) GO TO 28
      TERM2=TERV2*QLS*(DTIL/(APR*AP(L)*BP))**(0.5-0.5*EXM)
C     NOTE THAT RUU(1) AND RUU(NL)=0.
      EM12=.5*WML(L-1)/WML(L)-.5
      EM21=.5*WML(L)/WML(L-1)-.5
      EM23=.5*WML(L)/WML(L+1)-.5
      EM32=.5*WML(L+1)/WML(L)-.5
      VMU12=-.5*BMU(L-1)/WML(L)
      VMU21=.5*BMU(L-1)/WML(L-1)
      VMU23=-.5*BMU(L)/WML(L+1)
      VMU32=.5*BMU(L)/WML(L)
      DO 57 I=1,IS
      FFF=BP/BPA(I)
      ALDEN(I)=1.+RUU(L-1)*((1.+EM21)/FFF+VMU12)+RUU(L)*((1.+EM23)/
     $FFF+VMU32)
      DUML=RUU(L-1)*((1.+EM12)/FFF+VMU21)
      DUMR=RUU(L)*((1.+EM32)/FFF+VMU23)
      ALD=-RUU(L)*((1.+EM23)/FFF+VMU32)
      SMTT(I)=-DUMR*ALA(I,L+1)-ALD*ALA(I,L)
      CKINI(I)=CKINI(I)/ALDEN(I)
      DCR(I)=DUMR/ALDEN(I)
      DCL(I)=(1.+DUML)/ALDEN(I)
      ALPHI(I)=ALB(I,L-1)*DCL(I)+ALA(I,L+1)*DCR(I)
   57 ALPHZ(I)=ALPHI(I)
      HDN=1.
      DCR(ISP)=0.
      DCL(ISP)=1.
      IF(NEQ.NE.IS3) GO TO 28
      HDN=1.+RUU(L-1)*VMU12+RUU(L)*VMU32
      HTCOE=(RUU(L-1)*(1.+EM21)+RUU(L)*(1.+EM23))/HDN
      TCOE=(RUU(L-1)*CHI(L-1)+RUU(L)*CHI(L))/HDN
      DCL(ISP)=(1.+RUU(L-1)*VMU21)/HDN
      DCL(IS2)=RUU(L-1)*CHI(L-1)/HDN
      DCL(IS3)=RUU(L-1)*(1.+EM12)/HDN
      DCR(ISP)=RUU(L)*VMU23/HDN
      DCR(IS2)=RUU(L)*CHI(L)/HDN
      DCR(IS3)=RUU(L)*(1.+EM32)/HDN
      ALPHI(ISP)=0.
      DO 26 I=ISP,IS3
   26 ALPHI(ISP)=ALPHI(ISP)+DCL(I)*ALB(I,L-1)+DCR(I)*ALA(I,L+1)
   28 ALPHZ(ISP)=ALPHI(ISP)
      ALZISP=ALPHI(ISP)
      ALDEN(ISP)=HDN
      TERV2=TERV1*TERV2
      TERM2=TERM1*TERM2
      IF(KR7.GT.2)
     *WRITE(6,29) (ALPHI(I),I=1,ISP),APR
   29 FORMAT('  ALPHI,APR BEFORE  ' 7E14.8/(5X9E14.8))
      H=ALPHI(ISP)
      IF(L.EQ.2.AND.IS.EQ.NEQ) H=HH(1)
      IB=1
      STEP=1.
   30 FIB=IB-1
      CALL TLEFT(IARG)
      IF(KR7.GT.2)
     *WRITE(6,450) IARG
  450 FORMAT(10X,5HIARG= ,I4)
      IF(IARG.LT.20) INPCH=2
      DUM=1.-FIB*STEP
      DO 58 I=1,NEQ
   58 CKIN(I)=DUM*CKINI(I)
      IF(IB.NE.1.OR.IT.LE.2.OR.KR6.NE.2) GO TO 6114
      T=TL(L)
      PM=WML(L)*P
      DO6115 J=1,IS
      ALA(J,L)=AMAX1(ALA(J,L),1.E-30)
 6115 PLP(J)=ALOG(ALA(J,L)*PM)
 6114 IF(L.EQ.2) NFHS=NFH
C  ***************************************************
C  ***************************************************
C  ***************************************************
      CALL FLAME
C  ***************************************************
C  ***************************************************
C  ***************************************************
      NFHS=0
  207 FORMAT(1H ,22HFLAME PARAMETERS ITER=,I2,2X,4H IB=,I2)
      IF(KR7.EQ.4) KR7=KR77
      IF(ICON.EQ.0) GO TO 300
      IF(KR7.GT.1)
     *WRITE(6,207) ITER,IB
      IB=IB+IB
      IF(IB.GT.500) GO TO 301
      IF(IWSR.EQ.1) GO TO 522
      STEP=STEP/2.
      DO302 J=1,N
  302 PLP(J)=PPS(J)
      PM=PMS
      T=TTS
      GO TO 30
  300 DO303 J=1,N
  303 PPS(J)=PLP(J)
      TTS=T
      PMS=PM
      IF(IB.EQ.1) GO TO 310
      IB=IB-1
      IF(MOD(IB,2).EQ.1) GO TO 30
      IB=IB/2
      STFP=STEP*2.
      GO TO 30
  310 IF(KR7.GT.2)
     *WRITE(6,312) (ALPHI(I),I=1,ISP),APR
  312 FORMAT('  ALPHI,APR AFTER   ' 7E14.8/(5X9E14.8))
      IF(L.NE.2) GO TO 320
      DO 315 J=1,N
  315 PPI(J)=PLP(J)
      TINT=T
      PINT=PM
  320 CONTINUE
      DUM=1./PM
      IF(KR6.GE.2) DUM=DUM*82.057/T**.659/PM
      DO 326 J=1,MT
      PML(J,L)=PMR(J)*DUM
  326 RML(J,L)=PKR(J)/PKP(J)
      TL(L)=T
      RH(L)=PM/(82.057*T)
      IF(KR6.EQ.0.AND.IWSR.EQ.0) DTT(L)=DTT(L-1)+DS(L-1)*(AP(L-1)*RH(L-1
     *)+AP(L)*RH(L))*APR*.5
      IF(IWSR.EQ.1) DTT(L)=APR*AP(L)*RH(L)
      HH(L)=ALPHI(ISP)
      IF(KR6.NE.2) WML(L)=PM/P
      IF(KR7.GE.2.AND.INPCH.EQ.1)
     *WRITE(6,206)ITER,L,PM,T,(PP(J),J=1,N)
      IF(KR6.EQ.2.AND.NODRV.EQ.0) GO TO 323
      DO 322 I=1,NEQ
      ALB(I,L)=ALPHI(I)
      ALPHI(I)=ALA(I,L)
  322 ALA(I,L)=ALB(I,L)
      IF(KR6.NE.2) GO TO 27
  323 SS(L)=SS(L-1)+RTDS*DS(L-1)*.5
      RTDD=RH(L)*TL(L)**1.659
      RTDS=RTDD*SADB
      DLS(L)=RTDS*(DS(L)+DS(L-1))*.5
      SS(L)=SS(L)+RTDS*DS(L-1)*.5
      DTT(L)=DTT(L-1)+TTDS*DS(L-1)*.5
      TTDS=RH(L)*APR*AP(L)*RTDD
      DTT(L)=DTT(L)+TTDS*DS(L-1)*.5
      IF(INPCH.EQ.1.OR.KR7.EQ.0) GO TO 3212
      DUM=SQRT(DTIL/(BP*APR*AP(L)))
      DUM2=APR*AP(L)*(DS(L)+DS(L-1))*.5
      DO 3211 I=1,IS
      SMRT(I)=0.
      DO 3210 J=1,MT
 3210 SMRT(I)=SMRT(I)+(PMU(I,J)-RMU(I,J))*PMR(J)
      SMRT(I)=SMRT(I)*DUM2/PM*DUM
 3211 FCN(I)=ALPHI(I)*DUM
      WRITE(6,3214)  L,DLS(L)
 3214 FORMAT(1H0,4X,12HSTATION NO.=  ,I2,6X,12HNODAL WIDTH= ,E10.5,1X,4H
     *(CM)   )
      WRITE(6,3213) (NAMA(J),NAMB(J),J=1,IS)
 3213 FORMAT(10X,8(2X,2A4,2X)/15X,8(2X,2A4,2X)
     */20X,8(2X,2A4,2X)/25X,8(2X,2A4,2X))
      WRITE(6,501)(SMRT(I),I=1,IS)
      DO 3215  I=1,IS
 3215 SMTT(I)=SMTT(I)*DUM
      WRITE(6,501)  (SMTT(I),I=1,IS)
      WRITE(6,501)  (FCN(I),I=1,IS)
 3212 CONTINUE
      IF(NODRV.NE.0) GO TO 27
C
C       *** GENERATE  D(ALP(I))/D(ALPZ(K)) **
C
C     FIX INVERSE OF 'A' FOR REARRANGEMENTSIN KINETICS PACKAGE
C
      ISS=IS+2
      DO 106 I=1,ISS
      DO 106 J=1,ISS
  106 AA(I,J)=A(I,J)
      MZ=MT
      DO 110 MM=1,MT
      M=MA(MZ)
      IF(MP(M).GT.0) GO TO 110
      K=-MP(M)
      DO 109 J=1,IS
       IF(UNIT(J,K).EQ.0.) GO TO 109
      DO 108 I=1,ISS
  108 AA(I,K+2)=AA(I,K+2)-UNIT(J,K)*AA(I,J+2)
  109 CONTINUE
  110 MZ=MZ-1
C
C   --  LOAD D(DEP.VAR)/D(APR) IN COL 2 OF AA, THEN TO ZERO COL OF DAA
C                         AS D(ALP(I))/D(APR)
C
      IF(IFV.EQ.0) GO TO 114
      ALZISP=ALZISP-TCOE*ALPHI(IS2)-HTCOE*ALPHI(IS3)
      DUM=ALPHI(ISP)-ALZISP
      IF(MDOT.EQ.1)DUM=DUM-ALZISP+ALPHI(ISP)+(ALB(ISP.L-1)-ALPHI(ISP))/
     $ALDEN(ISP)
      DUM=DUM/APR
      DO 113  I=1.ISS
  113 AA(I.2)=AA(I.1)*DUM
      DO 112 J=1.IS
      DUM=ALPHI(J)-ALPHZ(J)
      IF(MDOT.EQ.1)DUM=DUM-ALPHZ(J)+(ALB(J.L-1)-ALPHI(J)*(1.-ALDEN(J)))/
     *ALDEN(J)
      DUM=DUM/APR
      DO 112  I=1.ISS
  112 AA(I.2)=AA(I.2)+AA(I.J+2)*DUM
  114 CONTINUE
C
C   --  SUM PARTIAL PRESSURE DERIVITIVES TO GET ALP DERIVITIVES  ---
C
      NZ=1-IFV                                                          RMK10057
      DO 125 K=NZ.ISP
      K2=K+2
      IF(K.EQ.ISP) K2=1
      DAA(IS3.K) =-PM*( ALPHI(IS3)*AA(2.K2) - T*CPTIL*AA(1.K2) )
      DAA(ISP.K)=-PM*(ALPHI(ISP)*AA(2.K2)-T*CPG*AA(1.K2))
      SUM=0.
      DO 115 I=1.IS
      DUM=PP(I)*AA(I+2.K2)
      DAA(ISP.K)=DAA(ISP.K)+DUM*HI(I)
      SUM=SUM + DUM*HI(I)*BPA(I)
  115 DAA(I.K)=-PM*ALPHI(I)*AA(2.K2)+DUM                                 RMK10057
      DAA(IS2.K) = AA(1.K2)*T*PM
      DAA(IS3.K)=DAA(IS3.K)+SUM/BP
      IF(ISP.GT.N)GO TO 125
      DO 124 J=ISP.N
      SUM=-TC(J)*AA(1.K2)
      DO 120 LL=1.IS
  120 SUM=SUM+VNU(J.LL)*AA(LL+2.K2)
      SUM=SUM*PP(J)
      DAA(ISP.K)=DAA(ISP.K)+SUM*HI(J)
      DAA(IS3.K) = DAA(IS3.K) + SUM*HI(J)*BPA(J)/BP                     RMK10057
      DO 124 I=1.IS
  124 DAA(I.K)=DAA(I.K)+VNU(J.I)*SUM
  125 CONTINUE
C
C   ))  DAA(I.K) IS NOW D(ALP(I))/D(ALPZ(K))   ((
      IF(L.NE.KAP.AND.L.NE.2) GO TO 127
      IF(KR7.LE.2) GO TO 6112
      DO 126 I=1.NEQ
  126 WRITE(6.44) (DAA(I.K).K=NZ.NEQ)
 6112 IF(IFV.EQ.0) GO TO 127
      TVECA=AA(1.2)
      TCON=(TKAP/T-1.)/PM
      DO 128 I=1,NEQ
         I2 = I + 2                                                     RMK10057
         IF (I .GE. ISP) I2 = 1                                         RMK10057
         TVEC(I) = AA(1,I2) * DCL(I)                                    RMK10057
         TVECR(I) = AA(1,I2) * DCR(I)                                   RMK10057
      IF(I.LE.ISP) TCON=TCON+AA(1,I2)*ALPHZ(I)
  128 CONTINUE                                                          RMK10057
C
C      ***SET UP RHS OF LINEAR EQUATION****
C
  127 DO 130  I=1,NEQ
      DAA(I,IS2) = DAA(I,ISP)                                           RMK10057
      DAA(I,IS3) = DAA(I,ISP)                                           RMK10057
      ALB(I,L) = ALPHI(I)
      ALPHI(I)=ALA(I,L)
      ALA(I,L)=ALB(I,L)
  130 DAR(I,L)=DAA(I,NUL)
      DO 138 J=1,NEQ
      DUMR=DCR(J)
      DUML=DCL(J)
  132 DO 139 I=1,NEQ
      IF (J .LE. ISP) ALA(I,L) = ALA(I,L) - ALPHZ(J) * DAA(I,J)         RMK10057
C
C        ****SET UP RIGHT HAND MATRIX*********
C
C
C     SET UP DIAGONAL AND LEFT HAND MATRIX   ****
C
      AA(I,J)=-DUML*DAA(I,J)
      UNIT(I,J)=0.
      IF(L.NE.NL) DAA(I,J)=-DUMR*DAA(I,J)
      IF(L.EQ.2) ARHM(I,J)=DAA(I,J)
C
C      ***** FOLD IN LEFT HAND MATRIX ****
C
      IF(IFV.EQ.1)DAR(I,L)=DAR(I,L)-AA(I,J)*DAR(J,L-1)
  139 ALA(I,L)=ALA(I,L)-AA(I,J)*ALA(J,L-1)
  138 UNIT(J,J)=1.0
      IF(L.EQ.2) GO TO 35
      CALL NTRAN(10,22)
      IF(LST.LT.0) STOP NTRANW
      DO 142 J=1,NEQ
      ARHM(J,NUL)=ALA(J,L)
      ARHM(J,NUL-1)=DAR(J,L)
      DO 142 IJ=1,NEQ
      IF(MDOT.EQ.1)
     $DAR(IJ,L-1)=DAR(IJ,L-1)+(ALPHI(J)-ALB(J,L))*ARHM(IJ,J)/APR
      DO 140 I=1,NEQ
  140 UNIT(I,J)=UNIT(I,J)-AA(I,IJ)*ARHM(IJ,J)
  142 IF(L.NE.NL) ARHM(IJ,J)=DAA(IJ,J)
C
C     *****  INVERT AND MULTIPY DIAGONAL BY RIGHT HAND MATRIX AND RHS
C
      IQ=0
      NN=NEQ+1+IFV
      IF(L.EQ.NL) NN=1+IFV
      NZ=-IFV
      CALL RERAY(NEQ.UNIT.0.ARHM(1.N7).NN.0.IQ)
      DO 34 J=1.NEQ
      ALA(J.L)=ARHM(J.NUL)
   34 DAR(J.L)=ARHM(J.NUL-1)
   35 IF(L.LT.NL-1) CALL NTRAN(10.1.JQQ.ARHM.LST)
   27 CONTINUE
C  -END OF MAJOR LOOP ON STATIONS
      IF(KR6.NE.2) GO TO 153
      IF(NODRV.NE.0) GO TO 153
      CALL NTRAN(10.6.-JQS)
C
C    )) FOLD RIGHT HAND MATRIX INTO ALA
C
      L = NL
      DO  150   LL  = 3. NL
      L=L-1
      IF(L.GE.NL-1) GO TO 148
      CALL NTRAN(10.2.JQQ.ARHM.LST)
      CALL NTRAN(10.22)
      CALL NTRAN(10.6.-JQS2)
      IF(LST.LT.0) STOP NTRANR
  148 DO 150 I=1.NEQ
      DO 150  J = 1.NEQ
      IF(IFV.EQ.1) DAR(I.L)=DAR(I.L)-ARHM(I.J)*DAR(J.L+1)
  150 ALA(I.L)=ALA(I.L)-ARHM(I.J)*ALA(J.L+1)
C
C  --  FOLD IN TEMPERATURE CONSTRAINT TO OBTAIN DELTA OF APR
C
      DA=0.
      IF(IFV.EQ.0) GO TO 153
      IF(IKAP.NE.0) GO TO 154
      L=KAP
      DEN=TVECA
      DO 151 I=1.NEQ
      TCON=TCON-TVECR(I)*ALA(I.L+1)-TVEC(I)*ALA(I.L-1)
  151 DEN=DEN+TVECR(I)*DAR(I.L+1)+TVEC(I)*DAR(I.L-1)
      DA=TCON/DEN
      GO TO 155
  154 DA=(TKAP-ALA(IKAP.KAP))/DAR(IKAP.KAP)
  155 CONTINUE
      DO 152 L=2.NL
      DO 152 I=1.NEQ
  152 ALA(I.L)=ALA(I.L)+DA*DAR(I.L)
  153 CONTINUE
C
C   MAJOR PRINTED OUTPUT
C
      IF(KR7.LE.1) GO TO 220
      WRITE(6.403) IT
      IF(NEQ.EQ.IS) WRITE(6.4011) (TL(J).J=1.NL)
      WRITE(6.400) IS.NL
      DO 402 I=1.NEQ
      IF(I.LE.IS) WRITE(6.404) NAMA(I).NAMB(I)
      IEN=I-IS+3
      IF(I.GT.IS) WRITE(6.404) NRA(IEN)
  404 FORMAT(2X.2A4)
      WRITE(6.401) (ALB(I.J).J=1.NL)
  402 WRITE(6,401) (ALA(I,J),J=1,NL)
  403 FORMAT(1H1,30X,34H* CONDENSED OUTPUT FOR ITERATION  ,I2,2H *  )
  400 FORMAT(1H0,17H((ALPHA(I,N),I=1,,I2,5H)N=1,,I2,1H)//
     *10X,26HPREDICTOR/CORRECTOR VALUES  //)
  401 FORMAT(1X,10E10.5/2X,10E10.5/3X,10E10.5/4X,10E10.5)
 4011 FORMAT(1H0,5X,14HTEMPERATURE(K)  /1X,10E10.5/2X,10E10.5/
     *3X,10E10.5/4X,10E10.5)
  220 CONTINUE
      DUMMX=0.
      DMAX=ABS(DA)/((1.85+SIGN(1.15,DA))*APR)
      SCALE=1.
      DO 160  L =2,NL
      DO 160  I=1,IS
      IF(ALB(I,L).LT.1.E-4) GO TO 159
      DUM = ALA(I,L) - ALB(I,L)
      DUM2=ABS(DUM/ALB(I,L))
      IF(DUM2.GT.DUMMX) DUMMX=DUM2
      DMAX=AMAX1(DMAX,ABS(DUM)/((2.9+SIGN(2.1,DUM))*ALB(I,L)))
      GO TO 160
  159 ALA(I,L)=AMAX1(ALA(I,L),ALB(I,L)*1.E-2)
  160 CONTINUE                                                  C
      IF (DMAX.LE.1.)  GO TO 175
      SCALE=1./DMAX
      DO 170  L= 2,NL
      DO 170 I = 1,NEQ
  170 ALA(I,L) = ALB(I,L) + SCALE*(ALA(I,L)-ALB(I,L))
  175 CONTINUE
      WRITE(6,1400) APR,DA,DUMMX,SCALE
 1400 FORMAT(1H0,15X,4HAPR=,E10.5,4X,5HDAPR=,E10.5,4X,16HMAX ALPHA ERROR
     *= ,E10.5,4X,5HDAMP=,E10.5    )
      DUM=1.+SCALE*DA/APR
      APR=APR+SCALE*DA
      IF(MDOT.EQ.0) GO TO 177
      BP=BP/DUM
      DO 176 I=1,IS
  176 BPA(I)=BPA(I)/DUM
  177 CONTINUE
      SPD=SQRT(.172E-4/(P*APH*AP(1)*BP))/RH(1)
  440 FORMAT(1H0,10X,16HFLAME SPEED PAR= ,E10.5,10X,12HFLAME SPEED=,E10.
     *5,2X,6HCM/SEC///)
 4401 FORMAT(1H0,9X,20HGRID COORDINATES(CM)  ,/)
      IF(IARG.LT.10) GO TO 301
      IF(INPCH.EQ.1.AND.KR6.GE.2) GO TO 1220
  522 WRITE(6,500) IT,NL
  500 FORMAT(1H1//30X,34H* GRID INFORMATION SUMMARY TABLE *////8X,10HITE
     *RATION=,
     *I4,8X,22HNUMBER OF GRID POINTS=,I4///)
      IF(KR6.GE.2) WRITE(6,440) APR,SPD
      WRITE(6,4401)
      WRITE(6,501)(SS(J),J=1,NL)
  501 FORMAT(10X,8(E10.5,2X)/15X,8(F10.5,2X)/20X,8(E10.5,2X)/25X,8(E10.5
     *,2X)/30X,8(E10.5,2X))
      WRITE(6,521)
  521 FORMAT(1H0,8X,31HNONDIMENSIONAL GRID INCREMENTS  )
      WRITE(6,501) (DS(J),J=1,NL)
      WRITE(6,803)
      WRITE(6,501) (UTT(J),J=1,NL)
  803 FORMAT(1H0,8X,9HTIME(SEC)/)
      WRITE(6,502)
  502 FORMAT(1H0,8X,16HENTHALPY(CAL/GM)/)
      WRITE(6,501) (HH(J),J=1,NL)
      WRITE(6,503)
  503 FORMAT(1H0,8X,14HTEMPERATURE(K)/)
      WRITE(6,501) (TL(J),J=1,NL)
      WRITE(6,504)
  504 FORMAT(1H0,8X,15HDENSITY(GM/CM3)/)
      WRITE(6,501) (RH(J),J=1,NL)
      WRITE(6,505)
  505 FORMAT(1H0,8X,23HSYSTEM MOLECULAR WEIGHT/)
      WRITE(6,501) (WML(J),J=1,NL)
      WRITE(6,506) N
  506 FORMAT(1H1/ 30X,19H* MOLE FRACTIONS OF    ,I4,2X,9HSPECIES *  ///)
      DO 507 I=1,N
      WRITE(6,508)NAMA(I),NAMB(I)
  508 FORMAT(9X,2A4/)
      DO 1507 J=1,NL
 1507 AX(J)=ALA(I,J)*WML(J)
  507 WRITE(6,501) (AX(J),J=1,NL)
      IF(KR7.EQ.0) GO TO 1220
      WRITE(6,509) MT
  509 FORMAT(1H1/20X,58H* NET FORWARD KINETIC PRODUCTION RATES(MOLE/(CC*
     1SEC)) FOR  ,I4,2X,11HREACTIONS * ///)
      DO510  I=1,MT
      WRITE(6,511) I
  511 FORMAT(9X,15HREACTION NUMBER,I4 )
  510 WRITE(6,501)(PML(I,J),J=1,NL)
      WRITE(6,512) MT
  512 FORMAT(1H1/20X,59H* RATIO OF FORWARD TO BACKWARD KINETIC PRODUCTIO
     *N RATES FOR ,I4,2X,11HREACTIONS *  ///)
      DO513 I=1,MT
      WRITE(6,511) I
  513 WRITE(6,501) (RML(I,J),J=1,NL)
      WRITE(6,908)
  908 FORMAT(1H1/20X,85H* KINETIC CONTRIBUTIONS TO INDIVIDUAL SPECIES(MO
     *LE/(CC*SEC)) REACTION/CONTRIBUTION  *       )
      DO907 JL=2,NL
      WRITE(6,910) JL
  910 FORMAT(1H0,10X,10HGRID POINT  ,I4)
      DO904 J=1,NEQ
      NCTT=0
      DO905  JJ=1,MT
      IF(RMU(J,JJ).EQ.0..AND.PMU(J,JJ).EQ.0.) GO TO 905
      NCTT=NCTT+1
      CTKN(NCTT)=(PMU(J,JJ)-RMU(J,JJ))*PML(JJ,JL)
      MCTT(NCTT)=JJ
  905 CONTINUE
      IF(NCTT.EQ.0) GO TO 904
      WRITE(6,906) NAMA(J),NAMB(J),(MCTT(JJ),CTKN(JJ),JJ=1,NCTT)
  906 FORMAT(10X,2A4,6(1H(,I2,1H/,E8.3,4H),  )/23X,6(1H(,I2,1H/,E8.3,4H)
     *,  )/28X,6(1H(,I2,1H/,E8.3,4H)      ))
  904 CONTINUE
  907 CONTINUE
 1220 CONTINUE
      IF(IWSR.EQ.1) GO TO 301
```

```
          IF(INPCH.EQ.2) GO TO 47
          NITM=IT+1
          IF(NOORV.NE.0) DMAX=1.
          IF(NITM.EQ.NIT.OR.DMAX.LE..001) INPCH=2
       45 CONTINUE
    C  ****END OF ITERATION LOOP
       47 IF(MOD(INA,2).EQ.0) GO TO 51
          PUNCH 210, TITLE
          PUNCH 2080, NL, IS, APR, BP
       54 PUNCH 48,  (DS(L),L=1,NL)
          PUNCH 4800,  (ALA(ISP,L),L=2,NL)
     4800 FORMAT(10E8.3)
          DO 46 I=1,IS
       46 PUNCH 48,  (ALA(I,L),L=2,NL )
       51 IF(INA.GT.3) GO TO 53
      301 STOP
          END
```

EPROP-ROUTINE

```
      SUBROUTINE  EPROP (L1,L2)
      PARAMETER JP=29,JE=28,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
     *+2,JSM=JS-1,JQQ=JQ*JQ
C     JX=NO. OF REACTIONS
C     JP=NO. OF SPECIES
C     JS=NO. OF STATIONS
C     JE=NO. OF ELEMENTS
      COMMON/EPRP/RUU(JS),BMU(JS),CHI(JS),ALA(JQ,JS)
     *,CPTIL,HTCOE,TCOE
      COMMON/F4/TITLE(20),RML(JX,JS),PML(JX,JS),AX(JS),WML(JS),RH(J
     *S),HH(JS),SS(JS),DTT(JS)
      COMMON/F3/ALPF(JQ),ALPE(JQ),ALPHZ(JQ),FLUX(JQ),PPI(JP),PPS(JP),
     *   ALB(JQ,JS),TL(JS),TWL(JS),AP(JS),AA(JE2,JE2),DUD(JQ),DUMB(JQ),
     *   ARHM(JQ,JQ),BPA(JQ),CKINI(JQ)
      COMMON/F1/RHS(JE2),A(JE2,JE2),E(JP),ALPHI(JQ),UNIT(JQ,JQ),
     *   VNU(JP,JE),RB(JP,2),RC(JP,2),RD(JP,2),RE(JP,2),RF(JP,2),
     *   TU(JP,2),PP(JP),PLP(JP),HI(JP),SB(JP),PPTC(JP),HOS(JP),
     *   TC(JP),CPF(JP),NAMA(JP),NAMB(JP),CPG,TW,HBC,PM,T,P,KR,KR6,KR7,
     *   N,IS,ISP,NEQ,MT,CKIN(JQ),H,PLN,ITER,ICON,IB,L,ICC,NFHS
     *,NRS(3),DQRDT,DQRDP(3),BP,PMW,FT,PW(JP)
      COMMON/LIN/ CPT(JP,50),HT(JP,50),GT(JP,50),HRF(JP),WM(JP),
     $   KNY,IQV(16,4),ALDEN(JP)
  100 FORMAT(2X,12E10.4)
      KR6S=KR6
      IS3=IS+3
      IF(NEQ.EQ.IS3) KR6S=3
      HTCOE=0.
      TCOE=0.
      KRS=KR
      KR6=-1
      KR=1
      IF(L1.EQ.1 ) GO TO 6
      CPTIL1=CPTILS
      U11=U11S
      U21=U21S
      CPG1=CPGS
      RL1=RL1S
    6 DO 1 L = L1,L2
      U22=0.
      U12=0.
      WML(L)=0.
      DO 2 J=1,IS
      U12=U12+ALA(J,L)/BPA(J)
      U22=U22+ALA(J,L)*WM(J)*BPA(J)
    2 WML(L)=WML(L)+ALA(J,L)
      WML(L)=1./WML(L)
      PM=P*WML(L)
      U12=U12*BP*WML(L)
      U22=U22/BP*WML(L)
      IF(KR7.GT.2) WRITE(6,100)U12,U22,WML(L),PM
      IF(L.NE.1)   GO TO 11
      KR6=1
      GO TO 12
   11 IF(KR6S.NE.3) GO TO 4
```

```
      H=ALA(ISP,L)
      T=AMAX1(T,ALA(IS+2,L))
   12 DO 3  J=1,IS
      ALPHI(J)=AMAX1(ALA(J,L),1.E-30)
    3 PLP(J)=ALOG(ALPHI(J)*PM)
C     ****************************************
C     ****************************************
      CALL FLAME
C     ****************************************
C     ****************************************
      IF(ICON.EQ.0) GO TO 7
      WRITE(6,9)
      STOP
    9 FORMAT(23H BAD CHEMISTRY IN EPROP   )
    7 CONTINUE
      RH(L)=PM/(82.057*T)
      TL(L)=T
      DO 13   J=ISP,IS3
   13 ALA(J,L)=ALPHI(J)
      IF(KR6S.NE.3) GO TO 8
      VMU3=0.
      DO 7001 I=1,IS                                                    RMK10107
      VMU3 = VMU3 +ALA(I,L)*BPA(I)
 7001 CONTINUE
      VMU3=VMU3/BP
      RL2=1.9865*.29*VMU3
    8 IF(L.NE.1)   GO TO 4
      U11S=U12
      U21S=U22
      IF(KR6S.NE.3) GO TO 5
      RL1S=RL2
      CPGS=CPG
      CPTILS=CPTIL
      GO TO 5
    4 CONTINUE
      RUU(L-1)=2./(U12+U11)
      BMU(L-1)=U22-U21
      IF(KR6S.NE.3) GO TO 10
      VMU12=-BMU(L-1)/WML(L)*0.5
      VMU21=BMU(L-1)/WML(L-1)*0.5
      EM12=(WML(L-1)-WML(L))/WML(L)*.5
      EM21=-EM12*WML(L)/WML(L-1)
      RLB=(RL2+RL1)/2.
      CHI(L-1)=RLB-0.5*(CPTIL*EM21+CPG*VMU12+CPTIL1*EM12+CPG1*VMU21)
      RL1=RL2
      CPG1=CPG
      CPTIL1=CPTIL
   10 U11=U12
      U21=U22
    1 CONTINUE
      NL=L2
      RUU(1)=0.
      RUU(NL)=0.
      CHI(NL)=0.
      BMU(NL)=0.
      WML(NL+1)=1.
    5 KR6=MIN0(KR6S,2)
```

```
      KR=KRS
      RETURN
      END
```

FLAME-ROUTINE

```
      SUBROUTINE FLAME
      PARAMETER JP=29.JE=28.JQ=JE+2.JX=70.JS=30.JE1=JE+1.JE2=JE+2.JQ1=JQ
     *+2
      DIMENSION BIG(JE).LL(JE)
      DIMENSION PKPE(JX).PKRF(JX)
      DIMENSION BIGN(JE)
      COMMON/EPRP/RUU(JS).BMU(JS).CHI(JS).ALA(JQ.JS)
     *.CPTIL.HTCOE.TCOE
      COMMON/F3/ALPF(JQ).ALPE(JQ).ALPHZ(JQ).FLUX(JQ).PPI(JP).PPS(JP).
     *   ALB(JQ.JS).TL(JS).TWL(JS).AP(JS).AA(JE2.JE2).DUD(JQ).DUMP(JQ).
     *  ARHM(JQ.JQ).BPA(JQ).CKINI(JQ)
      COMMON/F1/RHS(JE2).A(JE2.JE2).E(JP).ALPHI(JQ).UNIT(JQ.JQ).
     *   VNU(JP.JE).RB(JP.2).RC(JP.2).RD(JP.2).RE(JP.2).RF(JP.2).
     *   TU(JP.2).PP(JP).PLP(JP).HI(JP).SB(JP).PPTC(JP).HOS(JP).
     *   TC(JP).CPF(JP).NAMA(JP).NAMB(JP).CPG.TW.HBC.PM.T.P.KR.KR6.KR7.
     *   N.IS.ISP.NEQ.MT.CKIN(JQ).H.PLN.ITER.ICON.IB.L.ICC.NFHS
     *.NRS(3).DQRDT.DQRDP(3).BP.PMW.FT.PW(JP)
     $   .TERM2.TERV2.QRAD.TTV.PPV.TTT.PPP.FW(JP).CPWI(JP).ALFW(JE).CHIW
     $.  HTW.EXM.EXN.IH
      COMMON/F[illegible]/ THMU(JE1.JX).PPX(JX).RMU(JE.JX).PMU(JE.JX).PRMU(JE.JX).
     *   PKP(JX).PKR(JX).PMR(JX).XX(JX).DKPT(JX).FKF(JX).AFF(JX).
     *   EXK(JX).EAK(JX).RAT(JX)
     *  .MP(JX).MA(JX)
      COMMON /LIN/ CPT(JP.50). HT(JP.50). GT(JP.50). HRF(JP). WM(JP)
     *.KNY.IQV(16.4).ALDEN(JP)
      COMMON/HTL/SSS(JS).Q(JS).QLS.EGYDS
      DATA T/300./.R/1.9865/
      DATA NUL/0/
  200 FORMAT(1I1.E9.4.7E10.4)
  199 FORMAT(2I2)
  201 FORMAT(4H1 P=E12.4.10X.2HS=E12.4.10X4HVKT=5E12.4)
  202 FORMAT(4H1 P=E12.4.10X.2HH=E12.4.10X4HVKT=5E12.4)
      DO 3 J=1.N
      PLP(J)=AMAX1(PLP(J).-40.)
    3 PP(J)=EXP(PLP(J))
      ICB=0
      BUST=100.
      DAMP=1.0
   11 ITER=1
C     ICT IS NUMBER OF ITERATIONS AFTER CONVERGENCE BEFORE RETURN.
C     ITMX IS MAXIMUM NUMBER OF ITERATIONS
      ICT=0
      ITMX=50
      IMXP=1
      EMXP=1.E+10
      PLIM=2.3025851
C
C
C
   30 CONTINUE
      IF(ICC.GT.0) GO TO 806
C     JANAF THERMOCHEMICAL DATA SET
C     EVALUATE SPECIE STANDARD STATE FREE ENERGY AT PARTIAL PRESSURE
C     AND SYSTEM TEMPERATURE
```

```
      CPG=0.
      VA=ALOG(T/3000.)/1.9865
      VB=T-3000.
      VC=(T+3000.)/2.
      VD=T*3000.
      VE=VC/(VD*VD)
      VF=VB/1.9865
      RT=1.9865*T
      TSQ=T*T
      SUMP=0.
C     COMPUTE TEMPERATURE DEPENDENT THERMODYNAMIC PROPERTIES
      IF (KR7 .GT. 3) WRITE (6,801)
      DO 1 I=1,N
      J=2
      IF(T.LT.TU(I,1)) J=1
      CPF(I)=RC(I,J)+T*RD(I,J)+RE(I,J)/TSQ
      HI(I)=RB(I,J)+VB*(RC(I,J)+RD(I,J)*VC+RE(I,J)/VD)
      SB(I)=RF(I,J)+RC(I,J)*VA+VF*(RD(I,J)+RE(I,J)*VE)-PLP(I)
      CPG=CPG + PP(I)*CPF(I)
      SUMP=SUMP+PP(I)
      TC(I)=-HI(I)/RT
C     GET LN(KP) RELATIVE TO JANAF BASE
      E(I)=TC(I)+SB(I)
      IF (KR7 .GT. 3)
     *WRITE(6,805) NAMA(I),NAMB(I),CPF(I),HI(I),SB(I),TC(I),E(I),PP(I),P
     *LP(I)
      SB(I)=E(I)
    1 CONTINUE
      GO TO 808
  801 FORMAT(1H0,17HCPF,HI,SB,TC,E,PP)
C     EPA THERMOCHEMICAL DATA SET
  806 CPG=0.
      SUMP=0.
      RT=R*T
      J=T/100.
      RATIO=AMOD(T,100.)*.01
      DO 807 I=1,N
      CPF(I)=CPT(I,J)+RATIO*(CPT(I,J+1)-CPT(I,J))
      HI(I)=HT(I,J)+RATIO*(HT(I,J+1)-HT(I,J))
      G    =GT(I,J)+RATIO*(GT(I,J+1)-GT(I,J))
      SB(I)=(G+HI(I)/T)/R-PLP(I)
      HI(I)=HI(I)+HRF(I)
      TC(I)=-HI(I)/RT
      CPG=CPG+PP(I)*CPF(I)
      SUMP=SUMP+PP(I)
      SB(I)=TC(I)+SB(I)
      E(I)=SB(I)
      IF (KR7 .GT. 3)
     *WRITE(6,805) NAMA(I),NAMB(I),CPF(I),HI(I),SB(I),TC(I),E(I),PP(I),P
     *LP(I)
  807 CONTINUE
  800 FORMAT(1X,10E10.4/(5X,10E10.4))
  805 FORMAT(5X,2A4,8E10.4)
  808 IF(ITER.GT.1.OR.KR7.LE.2) GO TO 804
      WRITE(6,802)
  802 FORMAT(1H0,9HALPHI,VNU)
      DO803 I=1,IS
      WRITE(6,800)ALPHI(I)
  803 WRITE(6,800) (VNU(J,I),J=1,N)
C     GET LN(KP) FOR NON-BASE FORMATION REACTIONS
  804 ISP=IS+1
      IF(ISP.GT.N) GO TO 5
      DO 100 J=ISP,N
      DO 100 I=1,IS
      E(J)=E(J)-VNU(J,I)*E(I)
  100 TC(J)=TC(J)-VNU(J,I)*TC(I)
C
C     FORM CORRECTION COEFFICIENTS ARRAYS
C
    5 SUMH=0.
      CPTIL=0.
      DUM=HTCOE/BP
      DO 7  I=1,N
      CPTIL=CPTIL+PP(I)*CPF(I)*BPA(I)
      HOS(I)=HI(I)*PP(I)*(1.+DUM*BPA(I))
      SUMH=SUMH+HOS(I)
    7 CONTINUE
      CPTIL=CPTIL/BP
C----  CPG AND CPTIL ARE DIVIDED BY PM JUST BEFORE RETURN TO ACEF
      TCPMT=TCOE*PM*T
      A(1,1)=(CPG+HTCOE*CPTIL)*T+TCPMT
      A(1,2)=-PM*H+TCPMT
      RHS(1)=PM*H-SUMH-TCPMT
    6 RHS(2)=P-SUMP
C
C     COMPUTE ERRORS
      DO 111 I=1,IS
      DUM=PM*ALPHI(I)
      BIG(I)=AMAX1(0.,DUM)
      BIGN(I)=AMIN1(-PP(I),DUM)
      E(I)=DUM-PP(I)
      IF(ISP.GT.N) GO TO 111
      DO 110 J=ISP,N
      DUM=VNU(J,I)*PP(J)
      BIG(I)=AMAX1(BIG(I),-DUM)
      BIGN(I)=AMIN1(BIGN(I),-DUM)
  110 E(I)=E(I)-DUM
  111 CONTINUE
      ICON=1
      IF (KR7 .GT. 3)
     *WRITE(6,600) ITER,RHS(1),RHS(2),(E(I),I=1,IS)
  600 FORMAT(1H1,10HITERATION ,I2/20H  RHS1,RHS2,E,I=1,IS/(1X,10E10.3))
C
C     COMPUTE MATRIX AND RHS TO BE SOLVED FOR CORRECTIONS
C
   10 A(2,1)=0.
      A(2,2)=0.
      DO 14 I=1,IS
      A(I+2,2)=-PM*ALPHI(I)
      A(I+2,1)=0.
      A(1,I+2)=HOS(I)
      A(2,I+2)=PP(I)
      DO 12 II=1,IS
   12 A(II+2,I+2)=0.
```

```
      A(I+2,I+2)=PP(I)
   14 RHS(I+2)=E(I)
      IF(ISP.GT.N) GO TO 175
      DO 8 I=ISP,N
      A(1,1)=A(1,1)-HOS(I)*TC(I)
      PPTC(I)=PP(I)*TC(I)
      A(2,1)=A(2,1)-PPTC(I)
    8 CONTINUE
      A(2,2)=0.
      DO 120 I=1,IS
      DO 120 J=ISP,N
  120 A(I+2,1)=A(I+2,1)-VNU(J,I)*PPTC(J)
      DO 140 I=1,IS
      DO 140 J=ISP,N
      A(2,I+2)=A(2,I+2)+PP(J)*VNU(J,I)
  140 A(1,I+2)=A(1,I+2)+HOS(J)*VNU(J,I)
      DO 160 II=1,IS
      DO 160 I=1,IS
      DO 160 JJ=ISP,N
  160 A(II+2,I+2)=A(II+2,I+2)+PP(JJ)*VNU(JJ,II)*VNU(JJ,I )
      DO 9 I=ISP,N
      RHS(1)=RHS(1)-HOS(I)*E(I)
      PPTC(I)=PP(I)*E(I)
      RHS(2)=RHS(2)-PPTC(I)
    9 CONTINUE
      DO 170 I=1,IS
      DO 170 II=ISP,N
  170 RHS(I+2)=RHS(I+2)-VNU(II,I)*PPTC(II)
  175 ISS=IS+2
C     VOLUMETRIC HEAT LOSS MODELS
C
      IF(IABS(ICC).EQ.1.OR.IABS(ICC).EQ.4) GO TO 180
      DUM=PM*TERV2/ALDEN(ISP)
      IF(KR6.EQ.2) DUM=DUM*PM*T**0.659
      VQ=0.
      IF(IABS(ICC).EQ.2) GO TO 178
C     RADIATION HEAT LOSS
      CALL  RDFLX
      DO 176 J=1,3
      I=NRS(J)
  176 A(1,I+2)=A(1,I+2)+DUM*DQRDP(J)
      A(1,1)=A(1,1)+DUM*DQRDT
      VQ=QRAD
C     INPUT BULK HEAT LOSS
  178 IF(IABS(ICC).EQ.2) VQ=VQ+QLS
      VQ=VQ*DUM
      RHS(1)=RHS(1)-VQ
      A(1,1)=A(1,1)+VQ*TTV
      A(1,2)=A(1,2)+VQ*P
C     CONVECTIVE HEAT LOSS MODEL
  180 IF(IH-1) 188,182,184
C     NON-REACTIVE WALL
  182 VMU2=0.
      VMU1=0.
      WMU1=0.
      WMU3=0.
      CPTW=0.
      DO 183 I=1,N
      VMU1=VMU1+PP(I)/BPA(I)
      WMU1=WMU1+PP(I)*FW(I)
      VMU2=VMU2+PP(I)*BPA(I)*WM(I)
      V1=PP(I)/FW(I)
      CPTW=CPTW+V1*CPWI(I)
  183 WMU3=WMU3+V1
      CPTW=CPTW/PM
      WMU1=WMU1/P
      VMU1=VMU1/P*BP
      VMU2=VMU2/(P*BP)
      CHIW=1.9865*.29*WMU3/PM
      SCMN=(VMU2*P/(PM*1.344*VMU1))**(EXM-EXN)
      TERM3=SCMN/WMU1
      TERM=TERM2*TERM3*T**TTT*PM**PPP*(CPTW+CHIW)/ALDEN(ISP)
      WQ=TERM*(T-TW)
      RHS(1)=RHS(1)-WQ
      A(1,1)=A(1,1)+TTT*WQ+TERM*T
      A(1,2)=A(1,2)+PPP*WQ
      GO TO 188
  184 TERM=TERM2*T**TTT*PM**PPP
      DO 185 I=1,IS
      DUM=TERM/ALDEN(I)/FW(I)
      DUM1=DUM*PP(I)/PM
      WJ=DUM1-DUM*ALFW(I)
      RHS(I+2)=RHS(I+2)-WJ
      BIG(I)=AMAX1(BIG(I),-WJ)
      BIGN(I)=AMIN1(BIGN(I),-WJ)
      A(I+2,1)=A(I+2,1)+WJ*TTT
      A(I+2,2)=A(I+2,2)+WJ*PPP-DUM1
  185 A(I+2,I+2)=A(I+2,I+2)+DUM1
      IF(IH.EQ.3) GO TO 188
      DUM = TERM/ALDEN(ISP)
      HTB=0.
      CPTB=0.
      DO 186 I=1,N
      V1=PP(I)/(FW(I)*PM)
      V2=V1*HI(I)
      A(1,I+2)=A(1,I+2)+V2*DUM
      HTB=HTB+V2
  186 CPTB=CPTB+V1*CPF(I)
      WQ=DUM*(HTB-HTW+CHIW*(T-TW))
      RHS(1)=RHS(1)-WQ
      A(1,1)=A(1,1)+WQ*TTT+DUM*(CHIW+CPTB)*T
      A(1,2)=A(1,2)+WQ*PPP-DUM*HTB
  188 CONTINUE
      IF (KR7 .LE. 3) GO TO 508
      WRITE(6,502)
      DO501 I=1,ISS
  501 WRITE(6,500) ((A(I,J),J=1,ISS), RHS(I))
  500 FORMAT(1X,12F10.4/(2X,12F10.4))
  502 FORMAT(1X,20HA(I,J),RHS(I),BEFORE)
      WRITE(6,492) (BIG(I),I=1,IS)
     *,(BIGN(I),I=1,IS)
      WRITE(6,903)
  492 FORMAT(14H BIG(I),I=1,IS 10E10.4)
C     BEGINNING OF KINETICS PACKAGE
```

```
  508 IF(KR-2) 390,310,255
  255 IF(KR-5) 334,333,334
  333 DO 332 M=1,MT
      MA(M)=M
      DNT=THMU(ISP,M)
      DNE=0.
      IF(KR6.EQ.1) DNE=1.
      DO336 I=1,IS
      DNE=DNE-RMU(I,M)
  336 DNT=DNT+THMU(I,M)
      IF(DNT.GT.0.) DNE=DNE-1.
      FKF(M)=FKF(M)+DNE*4.4077187
      EXK(M)=EXK(M)+DNE
      IF(KR6.NE.2) GO TO 332
      FKF(M)=FKF(M)-4.4077187
      EXK(M)=EXK(M)+0.659
  332 XX(M)=FKF(M)
      KR=4
  334 ALPM=ALOG(PM)
      BE=0.
      IF (KR6.EQ.0) BE=1.0
      IF (KR6.EQ.2) BE=2.0
      DO 335 M=1,MT
      FKF(M)=XX(M)+BE*ALPM
      PPX(M)=THMU(ISP,M)*P
      DO 337 I=1,IS
  337 PPX(M)=PPX(M)+PP(I)*THMU(I,M)
      IF (PPX(M) .LE. 0.) GO TO 335
      FKF(M)=FKF(M)+ALOG(PPX(M))
      IF(NFHS.EQ.2) FKF(M)=1000.
  335 CONTINUE
  310 RT=1.9865*T
      RRT=1./RT
      IF(ICB.LE.0) BUMP=1.
      IF(PLIM.GT..1.OR.DAMP.GT..1) GO TO 314
      BUMP=BUST
      BUST=BUST*BUST
      ICB=10
      PLIM=2.3025851
      EMXP=1.E+10
  314 ICB=ICB-1
      DO 331 I=1,IS
      LL(I)=0
  331 OUD(I)=CKIN(I)*BUMP
C     CALCULATE RATES OF EACH REATION
      ALT=ALOG(T)
      DO 340 MM=1,MT
      M=MA(MM)
      MP(M)=1
      SUMD=0.
      SUMK=0.
      SUMR=0.
      SUMP=0.
      DO 315 I=1,IS
      IF(RMU(I,M).NE.0.) SUMR=SUMR+RMU(I,M)*PLP(I)
      PRMU(I,M)=PMU(I,M)-RMU(I,M)
      IF(PRMU(I,M).EQ.0.) GO TO 315
      SUMK=SUMK+PRMU(I,M)*SB(I)
      SUMD=SUMD+PRMU(I,M)*HI(I)
      PRMU(I,M)=PRMU(I,M)*DUD(I)
  315 CONTINUE
      AFF(M)=SUMK*RT
      DKPT(M)=SUMD*RRT
      VLK=FKF(M)+EXK(M)*ALT-EAK(M)*RRT
      PKRE(M)=SUMR+VLK
      PKPE(M)=PKRE(M)-SUMK
      DUM=AMAX1(PKRE(M),PKPE(M))-80.
      IF(DUM.LT.0.) GO TO 316
      VLK=VLK-DUM
      PKRE(M)=PKRE(M)-DUM
      PKPE(M)=PKPE(M)-DUM
  316 PKP(M)=EXP(PKPE(M))
      PKR(M)=EXP(PKRE(M) )
      PMR(M)=PKR(M)-PKP(M)
      RAT(MM)=AMAX1(PKP(M),PKR(M))
      IF (KR7 .LT. 3) GO TO 340
      WRITE(6,902) (PRMU(I,M),I=1,IS)
      WRITE(6,341) M,FKF(M),PPX(M),SUMK,SUMR,DKPT(M),VLK,EXK(M),EAK(M),
     *   PKR(M),PKP(M),PMR(M)
  902 FORMAT(1X,12E10.3)
  903 FORMAT(1H0,53HPRMU,M,FKF,PPX,SUMK,SUMR,DKPT,VLK,EXK,EAK,PKR,PKP,PM
     *R /)
  341 FORMAT(I3,2X,11E11.5)
  340 CONTINUE
      ISS=IS+2
      MX=MT
C     ORDER REACTIONS - FASTEST FIRST
      DO 453 J=1,1
  450 K=0
      DO 452 M=2,MX
      IF(RAT(M)-RAT(M-1)) 452,452,451
  451 K=MA(M)
      MA(M)=MA(M-1)
      MA(M-1)=K
      K=M-1
      DUM=RAT(M)
      RAT(M)=RAT(M-1)
      RAT(M-1)=DUM
  452 CONTINUE
      MX=K
      IF(K.GE.2) GO TO 450
  453 CONTINUE
C     INTRODUCE REACTIONS INTO CONSERVATION EQUATIONS
      DO 708 IK=1,MT
      M=MA(IK)
  507 K1=0
      TEST=2.
C     FIND K1 MASS BALANCE MOST EFFECTED BY REACTION
      DO 700 K=1,IS
      IF(LL(K).NE.0) GO TO 700
      BIGPP=BIG(K)
      BIGPN=-BIGN(K)
      IF(PRMU(K,M))703,700,702
  703 BIGPP=BIGN(K)
```

```
      BIGPN=-BIG(K)
  702 GP=BIGPP*1.E-3
      GN=BIGPN*1.E-3
      DUM=AMIN1(BIGPP/(PRMU(K,M)*PKP(M)+GP),BIGPN/(PRMU(K,M)*PKR(M)+GN))
      IF(DUM.GT.TEST) GO TO 700
      TEST=DUM
      K1=K
  700 CONTINUE
C     INTRODUCE REACTION INTO ALL MASS BALANCES
      IF(K1.GT.0) GO TO 701
      I1=1
      I2=IS
      GO TO 510
C     INTRODUCE REACTION ONLY INTO MOST IMPORTANT MASS BALANCE AFTER
C     REARRANGING
  701 K=K1
      DUM1=PRMU(K,M)
      IF (KR7 .GE. 3)
     *      WRITE (6,493) IK,M,RAT(IK),K,LL(K),PRMU(K,M),BIG(K)
     *,BIGN(K)
  493 FORMAT (2I3,E10.4/(2I3,3E10.4))
      LL(K)=IK
      MP(M)=-K
      DO704 I=1,IS
      UNIT(I,K)=0.
      IF(PRMU(I,M)) 705,704,705
  705 IF(I.EQ.K) GO TO 704
      DUM2=PRMU(I,M)/DUM1
      UNIT(I,K)=DUM2
      PRMU(I,M)=0.
      TST=ABS(CKIN(I))*BUMP*1.E-5
      DO 715 MM=1,MT
      IF(PRMU(K,MM).EQ.0.) GO TO 715
      IF(MP(MM).LT.0) GO TO 715
      PRMU(I,MM)=PRMU(I,MM)-DUM2*PRMU(K,MM)
      IF(ABS(PRMU(I,MM)).LT.TST) PRMU(I,MM)=0.
  715 CONTINUE
      DO 720  J=NUL,ISS
  720 A(I+2,J)=A(I+2,J)-DUM2*A(K+2,J)
      IF(DUM2.GT.0.) GO TO 721
      TST1=BIG(K)
      TST2=BIGN(K)
      GO TO 722
  721 TST1=BIGN(K)
      TST2=BIG(K)
  722 BIG(I)=AMAX1(BIG(I),-DUM2*TST1)
      BIGN(I)=AMIN1(BIGN(I),-DUM2*TST2)
  704 CONTINUE
      I1=K
      I2=K
  510 DUM=PMR(M)/PPX(M)
C     ADD REACTION TO MASS BALANCE(S)
      SUMD=0.
      DO 376 J=1,IS
      IF(RMU(J,M).NE.0.) SUMD=RMU(J,M)*PKR(M)
      IF(PMU(J,M).NE.0.) SUMD=SUMD-PMU(J,M)*PKP(M)
      IF(THMU(J,M).NE.0.) SUMD=SUMD+THMU(J,M)*DUM*PP(J)
      IF(SUMD.EQ.0.) GO TO 376
      DO375 I=I1,I2
  375 A(I+2,J+2)=A(I+2,J+2)-SUMD*PRMU(I,M)
      SUMD=0.
  376 CONTINUE
      SUMD=-PKP(M)*DKPT(M)-(EAK(M)/RT+
     *EXK(M))*PMR(M)
      DO 381 I=I1,I2
      IF(PRMU(I,M).EQ.0.) GO TO 381
      DUM1=PMR(M)*PRMU(I,M)
      A(I+2,2)=A(I+2,2)-DUM1*BE
      A(I+2,1)=A(I+2,1)+SUMD*PRMU(I,M)
      IF(I1.EQ.I2) GO TO 380
      BIG(I)=AMAX1(BIG(I),DUM1)
      BIGN(I)=AMIN1(BIGN(I),DUM1)
  380  RHS(I+2)=RHS(I+2)+DUM1
  381 CONTINUE
  708 CONTINUE
      IF (KR7 .GT. 3) WRITE(6,492) (BIG(I),I=1,IS)
     *,(BIGN(I),I=1,IS)
C     MODIFY MASS BALANCES AS REQUIRED TOWARD EQUILIBRIUM FORM.
      DO 750 I=1,IS
      IK=LL(I)
      IF(IK.EQ.0) GO TO 750
      M=MA(IK)
      LL(I)=M
      DUM=RAT(IK)*ABS(PRMU(I,M))
      BIGIE=BIG(I)
      IF(PMR(M)*PRMU(I,M).GT.0.)BIGIE=-BIGN(I)
      DUM1=DUM/(BIGIE+DUM*1.E-15)-1.0
      IF(DUM1.LT.0) GO TO 750
      BIG(I)=AMAX1(DUM,ABS(RHS(I+2)))
      IF(PMR(M)*PRMU(I,M)/RHS(I+2).LE.0.) GO TO 750
      DUM1=DUM1*DUM1
      WATE=DUM1/(10.+DUM1)
      FACT=RHS(I+2)*WATE
      DUM3=FACT/PRMU(I,M)
      DUM=FACT/PPX(M)
      IF (DUM3 .LE. 0.) GO TO 736
      DUM2=ALOG(DUM3+1.E-15)-PKPE(M)
      IF(DUM2.LT.20.)                DUM2=ALOG(1.+DUM3/PKP(M))
      GO TO 735
  736 DUM1=ALOG(-DUM3+1.E-15)-PKRE(M)
      IF(DUM1.LT.20.)                DUM1=ALOG(1.-DUM3/PKR(M))
  732 DO 730 J=1,IS
  730 A(I+2,J+2)= RMU(J,M)*FACT+A(I+2,J+2)
     *+DUM*THMU(J,M)*PP(J)
      DUM=-PKR(M)*PRMU(I,M)
      GO TO 745
  735 DO 740 J=1,IS
  740 A(I+2,J+2)= PMU(J,M)*FACT+A(I+2,J+2)
     *+DUM*THMU(J,M)*PP(J)
      A(I+2,1)=A(I+2,1)-FACT*DKPT(M)
      DUM= PKP(M)*PRMU(I,M)
      DUM1=DUM2
  745 A(I+2,1)=A(I+2,1)+(EXK(M)+EAK(M)/RT)*FACT
      A(I+2,2)=A(I+2,2)+FACT*BE
      IF(KR7.GT.3) WRITE(6.737)I.M.IK.DUM.DUM1.DUM2.FACT.RHS(I+2).WATE
  737 FORMAT(6X.3I4.6E12.7)
      RHS(I+2)=(FACT+DUM*WATE)*DUM1+RHS(I+2)-FACT
      BIG(I)=AMAX1(BIG(I).RAT(IK)*ABS(PRMU(I.M)))
      LL(I)=-M
  750 CONTINUE
      IF (KR7 .LE. 3) GO TO 390
      WRITE(6.497) (LL(I).I=1.IS)
      WRITE(6.498) (MA(I).I=1.MT)
  498 FORMAT(13H MA(I).I=1.IS.39I3/(1X.40I3))
  497 FORMAT(13H LL(I).I=1.IS.39I3/(1X.40I3))
      WRITE(6.499)
  499 FORMAT(1H0.43HA(I.J).RHS(I).AFTER KINET AND BEFORE INVERT)
      DO 904 I=1.ISS
  904 WRITE(6.500)((A(I.J).J=1.ISS).RHS(I))
C     END OF KINETICS PACKAGE
C
C     CONVERGENCE CHECK
  390 IF(ISP.GT.N) GO TO 393
      DO 16 I=ISP.N
      IF(ABS(E(I))-.001) 16.16.101
   16 CONTINUE
  393 CONTINUE
      IF(KR6.EQ.1.OR.NFHS.NE.0) RHS(1)=0.
      IF(ITER.EQ.1) GO TO 101
      IF(BUMP.GT.1.) GO TO 101
      IF(ABS(RHS(1)*T/A(1.1)).GT.0.1) GO TO 101
      IF(ABS(RHS(2))/P.GT. 0.00001) GO TO 101
      ESUM=0.
      DO 301 I=1.IS
      BIG(I)=AMAX1(BIG(I).-BIGN(I))
  301 ESUM=AMAX1(ESUM.ABS(RHS(I+2))/(BIG(I)+1.E-30))
      IF(ABS(ESUM)/PM.GT. .00001) GO TO 101
      ICT=ICT-1
      IF (ICT .LT. 0) ICON=0
      IF(KR7.LE.3) GO TO 101
      WRITE(6.497) (LL(I).I=1.IS)
      WRITE(6.498) (MA(I).I=1.MT)
      WRITE(6.903)
      DO 302 M=1.MT
      WRITE(6.902) (PRMU(I.M).I=1.IS)
      WRITE(6.341) M.FKF(M).PPX(M).SUMK.SUMR.DKPT(M).VLK.EXK(M).EAK(M).
     *   PKR(M).PKP(M).PMR(M)
  302 CONTINUE
  101 CONTINUE
C
C     NOW INVERT TO GET CORRECTIONS ON LN(T).PM.AND BASE SPECIE
C     PRESSURES
C
      J1=1
      IF(KR6.NE.1.AND.NFHS.EQ.0) GO TO 395
      DO394 I=NUL.ISS
      A(I.1)=0.
  394 A(1.I)=0.
      A(1.1)=1.0
  395 CONTINUE
      DO 391 I=NUL.ISS
      DUM=A(2,I)
      A(2,I)=A(ISS,I)
  391 A(ISS,I)=DUM
      DO392 I=1,ISS
      DUM=A(I,2)
      A(I,2)=A(I,ISS)
  392 A(I,ISS)=DUM
      DO 32 I=1,ISS
      DUM=A(I,I)
      IF(DUM) 343,49,343
  343 A(I,I)=1.0
      IP=I+1
      J1=J1+ICON
      IF(J1.GT.ISS) GO TO 311
      DO 31 J=J1,ISS
   31 A(I,J)=A(I,J)/DUM
  311 RHS(I)=RHS(I)/DUM
      IF(IP.GT.ISS) GO TO 33
      DO 32 K=IP,ISS
      DUM=A(K,I)
      A(K,I)=0.
      DO 321 J=J1,ISS
  321 A(K,J)=A(K,J)-DUM*A(I,J)
   32 RHS(K)=RHS(K)-DUM*RHS(I)
   33 IF(ICON.EQ.0) GO TO 36
      IP=ISS+1
      DO 35 I=1,ISP
      IP=IP-1
      DO 35 J=IP,ISS
   35 RHS(IP-1)=RHS(IP-1)-A(IP-1,J)*RHS(J)
      GO TO 38
   36 DO 37 I=1,ISP
      DO 37 J=1,I
      DUM=A(J,I+1)
      A(J,I+1)=0.
      DO 37 K=NUL,ISS
   37 A(J,K)=A(J,K)-DUM*A(I+1,K)
      DO 371 I=1,ISS
      DUM=A(2,I)
      A(2,I)=A(ISS,I)
  371 A(ISS,I)=DUM
      DO 372 I=1,ISS
      DUM=A(I,2)
      A(I,2)=A(I,ISS)
  372 A(I,ISS)=DUM
   38 CONTINUE
      DUM=RHS(2)
      RHS(2)=RHS(ISS)
      RHS(ISS)=DUM
      DO 189 I=1,IS
  189 E(I)=RHS(I+2)
      IF(ISP.GT.N) GO TO 191
      DO 190 I=ISP,N
      E(I)=E(I)-TC(I)*RHS(1)
      DO 190 II=1,IS
  190 E(I)=E(I)+VNU(I,II)*RHS(II+2)
  191 CONTINUE
```

```
      IF(NFHS.NE.0) A(1,1)=0.
C     NOW GET NON-BASE SPECIE CORRECTIONS
C
C
C     HERE IS WHERE TO DAMP CORRECTIONS IF NECESSARY
      IF(KR7.LE.3) GO TO 40
      WRITE(6,504)
      DO 503 I=1,ISS
  503 WRITE(6,500)((A(I,J),J=1,ISS),RHS(I))
  504 FORMAT(1H0,19HA(I,J),RHS(I),AFTER )
   40 DAMP=1.
      EMAX=1.E-30
      DO 15 I=1,N
      IF(ABS(EMAX).GT.ABS(E(I)))GO TO 42
      EMAX=E(I)
      IMAX=I
   42 DOM=PLP(I)-PLN
      IF(E(I)) 20,15,18
   18 DUM=(4.+4.*DOM)/(3.-DOM)
      GO TO 13
   20 DUM=(3.*DOM-4.)/(4.+DOM)
      IF(DUM) 13,15,15
   13 CONTINUE
   19 DAMP=AMIN1(DAMP,(DUM-DOM)/E(I))
   15 CONTINUE
      IF(E(IMXP)/EMXP.LT.-0.33) PLIM=PLIM/2.
      IF(MOD(ITER,2).EQ.0) EMXP=EMXP/EXP(PLIM)
      IF(ABS(1.-E(IMXP)/EMXP) .LT..25) PLIM=AMIN1(PLIM*2.,9.2103404)
      EMXP=EMAX
      IMXP=IMAX
      DAMP=AMIN1(DAMP,PLIM/(ABS(EMXP)))
      DAMP=AMIN1(DAMP,.4/AMAX1(ABS(RHS(1)),ABS(RHS(2)),.01))
      IF(DAMP.GT..99) GO TO 21
      DO 27 I=1,N
   27 E(I)=DAMP*E(I)
C     MAKE CORRECTIONS
   21 DO 28 I=1,N
      PLP(I)=PLP(I)+E(I)
      PP(I)=EXP(PLP(I))
   28 CONTINUE
      T=T/(1.-RHS(1)*DAMP)
      PM=PM+RHS(2)*PM*DAMP
      IF (KR7 .LT. 3) GO TO 48
      WRITE(6,505) DAMP,T,PM
  505 FORMAT(1H ,6HDAMP= ,F10.5,4H T= ,F10.5, 5H PM= ,E10.5 )
      WRITE(6,506) (PLP(I),I=1,N)
  506 FORMAT(5X,10E10.5)
   48 IF(ICON.GT.0) GO TO 45
      IF(IB.GT.1) RETURN
   52 SUMH=0.
      SUMHT=0.
      DO 53 I=1,N
      SUMH=SUMH+PP(I)*HI(I)
   53 SUMHT=SUMHT+PP(I)*HI(I)*BPA(I)
      DO55 I=1,IS
      ALPHI(I)=PP(I)
      IF(ISP.GT.N) GO TO 55
      DO50 J=ISP,N
   50 ALPHI(I)=ALPHI(I)+VNU(J,I)*PP(J)
   55 ALPHI(I)=ALPHI(I)/PM
      ALPHI(ISP)=SUMH/PM
      ALPHI(IS+3)=SUMHT/PM/RP
      ALPHI(IS+2)=T
      CPG=CPG/PM
      CPTIL = CPTIL/PM
      RETURN
   45 ITER=ITER+1
      IF(ITER.LT.ITMX) GO TO 30
      WRITE(6,47)
   47 FORMAT(1H0,27HALLOWED ITERATIONS EXCEEDED)
      RETURN
   49 ICON=1
   51 FORMAT(1H0,24HSINGULAR MATRIX IN FLAME)
      WRITE(6,51)
      KR7=4
      IF(ITER.GE.ITMX) RETURN
      KR7=MAX0(KR7,1)
      ITER=ITMX
      GO TO 30
      END
```

GETDAT-ROUTINE

```
      SUBROUTINF GETOAT(J)
      PARAMETER JP=29,JF=28,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
     *+2,JSM=JS-1,JQQ=JQ*JQ
      COMMON   /CARD1/   ISPECI(2),     XMW,      XHRF
      COMMON   /INUNIT/ INMAS
      COMMON /LIN/ CPT(JP,50), HT(JP,50), GT(JP,50), HRF(JP), WM(JP)
     *,KNY,IQV(16,4),ALDEN(JP)
      COMMON/F1/RHS(JE2),A(JE2,JE2),F(JP),ALPHI(JQ),UNIT(JQ,JQ),
     *   VNU(JP,JE),RB(JP,2),RC(JP,2),RD(JP,2),RE(JP,2),RF(JP,2),
     *   TU(JP,2),PP(JP),PLP(JP),HI(JP),SR(JP),PPTC(JP),HOS(JP),
     *   TC(JP),CPF(JP),NAMA(JP),NAMB(JP),CPG,TW,HBC,PM,T,P,KR,KR6,KR7,
     *   ,NRS(3),DQRDT,DQRDP(3),BP,PMW,FT,PW(JP)
      COMMON/F3/ALPF(JQ),ALPE(JQ),ALPHZ(JQ),FLUX(JQ),PPI(JP),PPS(JP),
     *   ALB(JQ,JS),TL(JS),TWL(JS),AP(JS),AA(JE2,JE2),DUD(JQ),DUMB(JQ),
     $   ARHM(JQ,JQ), BPA(JQ),CKINI(JQ)
      COMMON   /WANTS/   IWANT(3,JP),   NWANT,          XALPF(JP),
     $                   XALPE(JP)
         DIMENSION ZZ(JP,2)
      NAMA(J) = ISPECI(1)
      NAMB(J) = ISPECI(2)
      ALPF(J) = XALPF(J)
      ALPE(J) = XALPE(J)
      WM(J)=XMW
      IF(ICC.LT.0) GO TO 200
      HRF(J) = XHRF * 1000.
C              READ CP DATA
      READ (INMAS,20120) (CPT(J,K),K=1,50)
20120 FORMAT (5(1X, F9.4))
C              READ H DATA
      READ (INMAS,20120) (HT(J,K),K=1,50)
      DO 120 K=1,50
         HT(J,K) = HT(J,K) * 1000.
  120 CONTINUE
C              READ F DATA
      READ (INMAS,20120) (GT(J,K),K=1,50)
C              WRITE OUT DATA
      WRITE (6,20140) NAMA(J), NAMB(J),WM(J),HRF(J)
20140 FORMAT (10X, 2A4, 2(2X, F10.3))
      WRITE (6,20320) (CPT(J,K),K=1,50)
      WRITE (6,20320)  (HT(J,K),K=1,50)
      WRITE (6,20320)  (GT(J,K),K=1,50)
20320 FORMAT(5(1X,E12.5))
      GO TO 300
C
C              READ CUPVE FIT DATA
C
  200 CONTINUE
      DO 220 K=1,2
         READ (INMAS,20220) RA, RB(J,K), RC(J,K), RD(J,K), RE(J,K),
     *   RF(J,K), ZZ(J,K), TU(J,K)
20220    FORMAT (6E9.6, 2F6.0)
  220 CONTINUE
      WRITE (6,20140) NAMA(J), NAMB(J),WM(J)
```

```
         DO 240 K=1,2
            WRITE (6,20240) RA, RB(J,K), RC(J,K), RD(J,K), RE(J,K)
        *  ,HF(J,K), ZZ(J,K), TU(J,K), NAMA(J), NAMB(J)
   20240    FORMAT(5X, 6(E12.5,1X), 2(F6.0,1X), 2X, 2A4)
            RR(J,K) = RB(J,K) + RA
            RF(J,K) = RF(J,K) / 1.9865
     240 CONTINUE
     300 RETURN
         END
```

KINKIN-ROUTINE

```
      SUBROUTINE KININ
      PARAMETER JP=29,JE=28,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
     *+2
      INTEGER BLANK
      COMMON/F1/RHS(JE2),A(JE2,JE2),E(JP),ALPHI(JQ),UNIT(JQ,JQ),
     *   VNU(JP,JE),RB(JP,2),RC(JP,2),RD(JP,2),RE(JP,2),RF(JP,2),
     *   TU(JP,2),PP(JP),PLP(JP),HI(JP),SB(JP),PPTC(JP),HOS(JP),
     *   TC(JP),CPF(JP),NAMA(JP),NAMB(JP),CPG,TW,HAC,PM,T,P,KR,KR6,KR7,
     *   N,IS,ISP,NEQ,MT,CKIN(JQ),H,PLN,ITER,ICON,IB,L,ICC,NFHS
     *,NRS(3),DQRDT,DQRDP(3),BP,PMW,FT,PW(JP)
      COMMON/F2/ THMU(JE1,JX),PPX(JX),RMU(JE,JX),PMU(JE,JX),PRMU(JE,JX),
     *   PKP(JX),PKR(JX),PMR(JX),XX(JX),DKPT(JX),FKF(JX),AFF(JX),
     *   EXK(JX),EAK(JX),RAT(JX)
     * ,MP(JX),MA(JX)
      COMMON /LIN/ CPT(JP,50), HT(JP,50), GT(JP,50), HRF(JP), WM(JP)
     *,KNY,IQV(16,4),ALDEN(JP)
      DIMENSION NA(5),NT(2),NB(5),NTB(2),TB(2)
      DATA MLET/4HM   /
      DATA BLANK/4H    /
  451 FORMAT (2I3)
  452 FORMAT (5(A4,1X),F5.0,3E10.4,2(A4,F6.1))
C
      KIN=5
      KOUT=6
      AL10=ALOG(10)
  400 READ(KIN,451) MT
      WRITE(6,480) MT
  480 FORMAT(1H1,30X,25H* KINETIC REACTION DATA *   //15X,20HNUMBER OF R
     *EACTIONS=,I3/)
      WRITE(6,481)
  481 FORMAT(7X,1HM,13X
     *,8HREACTION,19X,  14HPRE EXP FACTOR,2X,8HTEMP EXP,6X,10HACTIVATION
     *,7X,28HINDIVIDUAL THIRD BODY EFFIC. /49X,11H(MOLE-CM-S),18X,11H(KC
     *AL/MOLE),6X,5HNAME1,5X,4HETB1,2X,5HNAME2,4X,4HETB2/)
      IFLAG=0
      DO 401 M=1,MT
      ISW=0
      RSUM=0
      PSUM=0
      READ (KIN,452) NA,FX,FKF(M),EXK(M),EAK(M),NT(1),TB(1),NT(2),TB(2)
      WRITE(6,482)M,NA,FKF(M),FX,EXK(M),EAK(M),NT(1),TB(1),NT(2),TB(2)
      DO 3 J=1,5
      NB(J)=BLANK
    3 CONTINUE
      NTB(1)=BLANK
      NTB(2)=BLANK
      FKF(M)=ALOG(FKF(M))+FX*AL10
  482 FORMAT(5X,I3,3X
     *          ,A4,1H+,A4,1H+,A4,3H--=,4X,A4,1H+,A4,6X,E10.4,1H+F3.0,2X
     *,F8.3,6
     *X,F10.4,8X,A4,4X,F6.3,4X,A4,F6.3)
      EAK(M)=1000.*EAK(M)
  305 DO 403 I=1,IS
      THMU(I,M)=0.
      RMU(I,M)=0.
      PMU(I,M)=0.
      IF (NA(3) .NE. NAMA(I).OR.NB(3).NE.NAMB(I)) GO TO 10
      THMU(I,M)=1.
      NA(3)=BLANK
   10 DO 402 J=1,2
      IF(NT(J).NE. NAMA(I).OR.NTB(J).NE.NAMB(I))GO TO 11
      THMU(I,M)=TB(J)
      NT(J)=BLANK
   11 IF(NA(J).NE.NAMA(I).OR.NB(J).NE.NAMB(I))GO TO 12
      RMU(I,M)=PMU(I,M)+1.
      NA(J)=BLANK
   12 IF(NA(J+3).NE.NAMA(I).OR. NB(J+3).NE.NAMB(I))GO TO 13
      PMU(I,M)=PMU(I,M)+1.
      NA(J+3)=BLANK
   13 DO 402 L=ISP,N
      IF(NA(J+3).NE.NAMA(L).OR.NB(J+3).NE.NAMB(L))GO TO 402
      PMU(I,M)=PMU(I,M)+VNU(L,I)
      NA(J+3)=BLANK
  402 CONTINUE
      RSUM=RMU(I,M)*WM(I)+RSUM
      PSUM=PMU(I,M)*WM(I)+PSUM
  403 CONTINUE
      THMU(ISP,M)=0.
      IF(NA(3).EQ.MLET) THMU(ISP,M)=1.
      IF(NA(3).EQ.MLET) NA(3)=BLANK
      ISW=-ISW
      DO 410 K=1,7
      IF (NA(K) .EQ. BLANK) GO TO 410
      IF(KNY.EQ.0.OR.ISW.EQ.-1) GO TO 7
      DO 300 II=1,KNY
      DO 300 JJ=1,4,2
      IF(NA(K).EQ.IQV(II,JJ).AND.IQV(II,JJ+1).EQ.NB(K)) GO TO 301
  300 CONTINUE
      GO TO 7
  301 J1=4-JJ
      J2=5-JJ
      NA(K)=IQV(II,J1)
      NB(K)=IQV(II,J2)
      ISW=1
      GO TO 410
    7 WRITE(6,409) NA(K),M
  409 FORMAT(5X,A4,13H OF EQUATION I3,28H IS NOT IN THE SPECIES TABLE)
      IFLAG=1
  410 CONTINUE
      IF(ISW.EQ.1) GO TO 305
      IF(ABS(RSUM-PSUM).LE. .0001*RSUM) GO TO 401
      WRITE(6,406) M
  406 FORMAT(66H SUM OF MOLECULAR WEIGHTS INDICATES IMBALANCE IN KINETIC
     * EQUATION I3)
      IFLAG = 1
  401 CONTINUE
      IF (IFLAG .EQ. 1) STOP
      RETURN
      END
```

OBTAIN-ROUTINE

```
      SUBROUTINE OBTAIN
      PARAMETER JP=29,JE=28,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
     *+2,JSM=JS-1,JQQ=JQ*JQ
      COMMON/F3/ALPF(JQ),ALPE(JQ),ALPHZ(JQ),FLUX(JQ),PPI(JP),PPS(JP),
     *   ALB(JQ,JS),TL(JS),TWL(JS),AP(JS),AA(JE2,JE2),DUD(JQ),DUMB(JQ),
     $   ARHM(JQ,JQ), BPA(JQ),CKINI(JQ)
      COMMON   /INUNIT/ INMAS
      COMMON /LIN/ CPT(JP,50), HT(JP,50), GT(JP,50), HRF(JP), WM(JP)
     *,KNY,IQV(16,4),ALDEN(JP)
      COMMON   /WANTS/   IWANT(3,JP),   NWANT,          XALPF(JP),
     $                   XALPE(JP)
      DIMENSION LNGTH(2)
      COMMON  /CARD1/  ISPECI(2),  XMW,  XHRF
      COMMON /F1/RHS(JE2),A(JE2,JE2),E(JP),ALPHI(JQ),UNIT(JQ,JQ),
     *  VNU(JP,JE),RB(JP,2),RC(JP,2),RD(JP,2),RE(JP,2),RF(JP,2),
     *    TU(JP,2),PP(JP),PLP(JP),HI(JP),SB(JP),PPTC(JP),HOS(JP),
     *   TC(JP),CPF(JP),NAMA(JP),NAMB(JP),CPG,TW,HBC,PM,T,P,KR,KR6,KR7,
     *   N,IS,ISP,NEQ,MT,CKIN(JQ),H,PLN,ITER,ICON,IB,L,ICC,NFHS
     *  ,NRS(3),DQRDT,DQRDP(3),BP,PMW,FT,PW(JP)
      DATA LNGTH/ 2, 30 /
      DATA IEND/3HEND/
      OK = 0
      DO 9 I=1,NWANT
      IWANT(1,I)=0
    9 CONTINUE
C  CURVE FIT DATA ASSIGNED TO UNIT 11
C  TABULAR   DATA ASSIGNED TO UNIT 12
      INMAS =12
      IF(ICC.LT.0) INMAS=11
      REWIND INMAS

C     ORIGINALLY COMPAR

      NLNGTH = LNGTH(2)
      IF(ICC.LT.0) NLNGTH=LNGTH(1)
      MATCH = 0
      IEOF = 0
         WRITE(6, 300)
  300 FORMAT(1H1,30X,24H* THERMOCHEMISTRY DATA *  ,/)

      IF(INMAS.EQ.11) WRITE (6,10)
   10 FORMAT(1H0,15X,59HCURVE FIT OF DATA IN FORM CP=RB+RC*T+RD/(T*T) (C
     *AL/(MOLE*K)//7X,12H HF(CAL/MOL),2X, 10HH(CAL/MOL),5X,2HRB,11X,2HRC
     *,11X,2HRD,7X,12HS(CAL/MOL/K),6X,5HTU(K),4X,4HNAME   /)
      IF(INMAS.EQ.12) WRITE (6,11)
   11 FORMAT(1H0,15X,12HTABULAR DATA/12X, 4HNAME, 8X, 2HMW,6X,11HHF(CAL/
     *MOL)/15X,   78HCP(CAL/(MOL*K)),H(CAL/MOL),F(CAL/(MOL*K) GIVEN EVER
     *Y 100K FROM 100 TO 5000K     )
C     ORIGINALLY GETSPE(IEOF)

      READ(INMAS,4) IHDG
    4 FORMAT(A2)
    3 READ(INMAS,1) ISPECI,XMW,XHRF
    1 FORMAT(10X,2A4,2X,2F10.0)
```

```
      IF (ISPECI(1) .EQ. IEND) IEOF = 1

      IF (IEOF .NE. 0) GO TO 200
      IF(KNY.EQ.0) GO TO 150
      DO 2 I=1,KNY
      DO 2 J=1,4,2
      IF(ISPECI(1).NE.IQV(I,J))GO TO 2
      IF (ISPECI(2).NE.IQV(I,J+1))GO TO 2
      J1=4-J
      ITEST1=IQV(I,J1)
      J2=5-J
      ITEST2=IQV(I,J2)
      GO TO 150
    2 CONTINUE
  150 DO 160 I=1,NWANT
          IF (IWANT(1,I) .NE. 0) GO TO 160
              DO 120 J=1,2
      IF(IWANT(J+1,I).EQ.ISPECI(J)) GO TO 120
  110 IF(IWANT(2,I).NE.ITEST1) GO TO 160
      IF(IWANT(3,I).NE.ITEST2)GO TO 160
  120         CONTINUE
              MATCH = MATCH + 1
              IWANT(1,I) = MATCH
              CALL GETDAT(I)
              IF (MATCH .EQ. NWANT) GO TO 200
      GO TO 3
  160 CONTINUE

C     ORIGINALLY GETDUM(NLNGTH)

      DO 8 I=1,NLNGTH
          READ (INMAS,20100) IDUM
20100     FORMAT (A1)
    8 CONTINUE

      GO TO 3

C     ORIGINALLY CHECK(OK)

  200 DO 5 I=1,NWANT
      IF(IWANT(1,I).NE.0) GO TO 5
      WRITE(6,6)(IWANT(J,I),J=2,3)
    6 FORMAT(1H0, 39H*** NO DATA IN SPECIES MASTER FILE FOR , 2A4,
     $            4H ***
     $)
          OK = OK + 1
    5 CONTINUE

      IF(OK.EQ.0) GO TO 7
          WRITE (6,20120)
20120     FORMAT (1H0, 47H*** PROGRAM STOPPED IN OBTAIN - UNKNOWN SPECIES
     $,           14H REQUESTED ***
     $)
          STOP
    7 RETURN
      END
```

<u>RDFLX-ROUTINE</u>

```
    SUBROUTINE RDFLX
    PARAMETER JP=29,JE=2A,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
   *+2,JSM=JS-1,JQQ=JQ*JQ
    COMMON/F1/RHS(JE2),A(JE2,JE2),E(JP),ALPHI(JQ),UNIT(JQ,JQ),
   *VNU(JP,JE),RB(JP,2),RC(JP,2),RD(JP,2),RE(JP,2),RF(JP,2),
   *TU(JP,2),PP(JP),PLP(JP),HI(JP),SB(JP),PPTC(JP),HOS(JP),
   *TC(JP),CPF(JP),NAMA(JP),NAMB(JP),CPG,TW,HBC,PM,T,P,KR,KR6,KR7,
   *   N,IS,ISP,NEQ,MT,CKIN(JQ),H,PLN,ITER,ICON,IB,L,ICC,NFHS
   *,NRS(3),DQRDT,DQRDP(3),BP,PMW,FT,PW(JP)
   $,  TERM2,TERV2,QRAD,TTV,PPV,TTT,PPP,FW(JP),CPWI(JP),ALFW(JE),CHIW
   $,  HTW,EXM,EXN,IH
    COMMON/HTL/SSS(JS),Q(JS),QLS,EGYDS
    DIMENSION  TEMP(12), XKPCO2(12), XKPH20(12), XKPCO(12)
    DATA TEMP/ 400.,600.,800.,1000.,1200.,1400.,1600.,1800.,2000.,2200
   *.,2400.,2600./
    DATA XKPCO2/0.11431,0.12744,0.10779,0.08005,0.057615,0.04147,0.030
   *2,0.022343,0.016831,0.012884,0.010023,0.0079071/
    DATA XKPH20/0.4721,0.21435,0.10484,0.05742,0.03554,0.02378,0.0168,
   *0.01233,0.00933,0.007238,0.00573,0.004611/
    DATA XKPCO/0.003698,0.008107,0.008589,0.007313,0.005764,0.004419,
   *0.00336,0.002549,0.001941,0.001482,0.0011345,0.000877/
    DATA SIGMA/1.356E-12/
    IF(T.LT.400.) GO TO 10
    J = T / 200.0
    J=J-1
    RATIO=AMOD(T,200.)*0.005
    IF(T.GE.2600.) J=11
    PKCO2=XKPCO2(J)+RATIO*(XKPCO2(J+1)-XKPCO2(J))
    PKH20=XKPH20(J)+RATIO*(XKPH20(J+1)-XKPH20(J))
    PKCO =XKPCO(J) +RATIO*(XKPCO(J+1)-XKPCO(J))
    I1 = NRS(1)
    I2 = NRS(2)
    I3 = NRS(3)
    PPI1=0.
    PPI2=0.
    PPI3=0.
    IF(NRS(1).GT.0) PPI1=PP(I1)
    IF(NRS(2).GT.0) PPI2=PP(I2)
    IF(NRS(3).GT.0) PPI3=PP(I3)
    SUMKP=PPI1*PKCO2+PPI2*PKH20+PPI3*PKCO
    FAC=4.0*SIGMA*T**4
    QRAD=FAC*SUMKP
    T1=(XKPCO2(J+1)-XKPCO2(J))/200.
    T2=(XKPH20(J+1)-XKPH20(J))/200.
    T3=(XKPCO (J+1)-XKPCO (J))/200.
    DKPDT=PPI1*T1+PPI2*T2+PPI3*T3
C
    DQRDT=QRAD*(4.0+T*DKPDT/SUMKP)
C
    DQRDP(1)=FAC*PPI1*PKCO2
    DQRDP(2)=FAC*PPI2*PKH20
    DQRDP(3)=FAC*PPI3*PKCO
C
    RETURN
   10 CONTINUE
      QRAD=0.
      DQRDT=0.0
      DQRDP(1)=0.0
      DQRDP(2)=0.0
      DQRDP(3)=0.0
      RETURN
      END
```

READIN-ROUTINE

```
      SUBROUTINE READIN
C              READS IN THE CARD(S) INDICATING THE SPECIES AND
C              THE ALPF AND ALPE VALUES THE PROGRAM WILL USE
      PARAMETER JP=29,JE=28,JQ=JE+2,JX=70,JS=30,JE1=JE+1,JE2=JE+2,JQ1=JQ
     *+2,JSM=JS-1,JQQ=JQ*JQ
      DIMENSION      ISPECI(2)
      COMMON/F3/ALPF(JQ),ALPE(JQ),ALPHZ(JQ),FLUX(JQ),PPI(JP),PPS(JP),
     *   ALB(JQ,JS),TL(JS),TWL(JS),AP(JS),AA(JE2,JE2),DUD(JQ),DUMB(JQ),
     *   ARHM(JQ,JQ),BPA(JQ),CKINI(JQ)
      COMMON   /WANTS/   IWANT(3,JP),   NWANT,           XALPF(JP),
     $                   XALPE(JP)
      COMMON /LIN/ CPT(JP,50), HT(JP,50), GT(JP,50), HRF(JP), WM(JP)
     *,KNY,IQV(16,4),ALDEN(JP)
      DATA      IEND /3HEND/
      JMAX = JP
      J = 1
         WRITE(6, 10)
   10 FORMAT(1H1,15X,70H* SPECIES INITIAL MOLE FRACTIONS,FIRST GUESSES,A
     *ND DIFFUSION FACTORS *    ,/)
      WRITE (6,20090)
20090 FORMAT(/, 15X, 6HSPECIE,18X, 4HALPF, 16X, 4HALPE, 10X
     *,16HDIFFUSION FACTOR/)
  100 READ (5,20100)ISPECI,KNY,XF,XE,XBP
20100 FORMAT(2A4,I2,2E10.3,F10.4)
      IF (ISPECI(1) .EQ. IEND) GO TO 180
      WRITE(6,20120) ISPECI,XF,XE,XBP
20120 FORMAT(16X,2A4,12X,E10.3,10X,E10.3,10X,F10.4)
      IF (J .GT. JMAX) GO TO 200
         DO 140 I=1,2
            IWANT(I+1,J) = ISPECI(I)
  140    CONTINUE
         XALPF(J) = XF
         XALPE(J) = XE
      BPA(J)=XBP
         J = J + 1
  160 GO TO 100
  180 NWANT = J - 1
      IF(KNY.EQ.0)GO TO 220
      KNY=4*KNY
      READ(5,2)((IQV(I,J),J=1,4),I=1,KNY)
    2 FORMAT(8(A4,A4,2X))
      WRITE(6,6)
    6 FORMAT(5X,54HTHE FOLLOWING PAIRS OF NAMES ARE CONSIDERED EQUIVALEN
     *T,/,
     *T11,1H",T21,1H",T31,1H",T41,1H",T51,1H",T61,1H",T71,1H",T81,1H")
      WRITE(6,7)((IQV(I,J),J=1,4),I=1,KNY)
    7 FORMAT(10X,2A4,2X,2A4,2X,2A4,2X,2A4,2X,2A4,2X,2A4,2X,2A4,
     *2X,2A4,2X)
      GO TO 220
C
C              MORE THAN JMAX SPECIES REQUESTED
C
  200 WRITE (6,20200) JMAX
20200 FORMAT (43H0*** PROGRAM STOPPED IN READIN -- MORE THAN, I5,
     $          22H SPECIES REQUESTED ***
     $)
 210 READ (5,20100) IDUM
     IF (IDUM .NE. IEND) GO TO 210
 220 RETURN
     END
```

RERAY-ROUTINE

```
      SUBROUTINE RERAY(N,C,NN,D,NNN,LS,IS)
C     DIRECT INVERSION PROCEDURE  --  C IS REPLACED BY C**-1                 1
      PARAMETER  JE=28,JE2=JE+2
      DIMENSION D(JE2,1),C(JE2,1)
      DIMENSION SD(JE2),L(JE2),S(JE2),LL(JE2),LLL(JE2),LS(1)
      KOUT=6
      N1=N+1
      NP=N+NN
      DO 11 I=1,NP
      LLL(I)=I
      IF(LS(1)) 113,113,112
  112 L(I)=LS(I)
      GO TO 11
  113 L(I)=I
   11 CONTINUE
      IX=-1
      IF(IS+2) 111,109,111
  106 FORMAT(11H  L(I),I=1,I3,5X (30I3))
  107 FORMAT(15H  ((C(I,J),J=1,I3,12H),(D(J),J=1,I3, 6H),I=1,I3,15H)  BE
     1FORE RERAY)
  108 FORMAT(2X  11E10.3/(12X  10E10.3))
  109 WRITE(KOUT,107) NP,NNN,N
      WRITE(KOUT,106)NP,(L(I),I=1,NP)
      IX=0
      DO 110 I=1,N
  110 WRITE(KOUT,108)(C(I,J),J=1,NP),(D(I,J),J=1,NNN)
  111 IS=-1
C     TRIANGULATE MATRIX
      DO 15 I=1,N
      DO 160 M=1,NP
  160 S(M)=ABS(C(I,M))
      IF(IS) 18,16,16
   18 IS=0
      SD(1)=1.
      GO TO 12
C     REDUCE ROW I BY PRECEEDING ROWS
   16 DO 17 J=2,I
      K=L(J-1)
      DIV=-C(I,K)
      IF(DIV) 161,17,161
  161 C(I,K)=0.
      DO162 M=1,NP
      DIVC=DIV*C(J-1,M)
      S(M)=AMAX1(S(M),ABS(DIVC))
  162 C(I,M)=C(I,M)+DIVC
      IF(NNN) 17,17,163
  163 DO 164 M=1,NNN
  164 D(I,M)=D(I,M)+DIV*D(J-1,M)
   17 CONTINUE
C     SEEK MAXIMUM PIVOT
   12 DIV=0.
      K=L(I)
      J=I
      DO 13 JJ=I,N
      M=L(JJ)
      IF(ABS (C(I,M))-DIV)13,13,121
  121 DIV=ABS (C(I,M))
      K=M
      J=JJ
   13 CONTINUE
      SD(I)=DIV/S(K)
      L(J)=L(I)
      L(I)=K
      IF(SD(I)-1.E-8) 131,131,14
C     SINGULAR MATRIX RETURN
  131 IS=-I
      WRITE(KOUT,132) I,K
      C(I,K)=1.E+30
      S(K)=1.0
      GO TO 12
  132 FORMAT(115X2I3)
   14 DIV=C(I,K)
      C(I,K)=1.0
      K=LLL(J)
      LLL(J)=LLL(I)
      LLL(I)=K
      LL(K)=I
C     NORMALIZE ROW
      IF(NNN) 143,143,141
  141 DO 142 J=1,NNN
  142 D(I,J)=D(I,J)/DIV
  143 DO 15 J=1,NP
   15 C(I,J)=C(I,J)/DIV
      IF(IX) 152,150,152
  151 FORMAT(24H PIVOT ROW/COL/RES,RATIO 5(I4,1H/I3,1H/E9.2,1H,))
  150 WRITE(KOUT,151) (I,L(I),SD(I),I=1,NP)
C     DIAGONALIZE MATRIX
  152 NM=N-1
      DO 20 I=1,NM
      K=L(I+1)
      DO 20 J=1,I
      DIV=-C(J,K)
      IF(DIV)19,20,19
   19 C(J,K)=0.
      IF(NNN) 191,191,192
  192 DO 193 M=1,NNN
  193 D(J,M)=D(J,M)+DIV*D(I+1,M)
  191 DO 201 M=1,NP
  201 C(J,M)=C(J,M)+DIV*C(I+1,M)
   20 CONTINUE
C     INTERCHANGE COLUMNS
      DO 30 II=1,NP
      I=II
   21 J=L(I)
      L(I)=I
      IF(J-I)22,30,22
   22 IF(IS)25,23,25
   23 DO 24 M=1,N
      S(M)=C(M,I)
   24 C(M,I)=C(M,J)
      IS=I
```

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```
      I=J
      GO TO 21
   25 IF(IS-J)26,28,26
   26 DO 27 M=1,N
   27 C(M,I)=C(M,J)
      I=J
      GO TO 21
   28 DO 29 M=1,N
   29 C(M,I)=S(M)
      IS=0
   30 CONTINUE
C     INTERCHANGE ROWS
      DO 40 II=1,N
      I=II
   31 J=LL(I)
      LL(I)=I
      IF(J-I)32,40,32
   32 IF(IS)35,33,35
   33 DO 34 M=1,NP
      S(M)=C(I,M)
   34 C(I,M)=C(J,M)
      IF(NNN) 343,343,341
  341 DO 342 M=1,NNN
      SD(M)=D(I,M)
  342 D(I,M)=D(J,M)
  343 IS=I
      I=J
      GO TO 31
   35 IF(IS-J)36,38,36
   36 DO 37 M=1,NP
   37 C(I,M)=C(J,M)
      IF(NNN) 373,373,371
  371 DO 372 M=1,NNN
  372 D(I,M)=D(J,M)
  373 I=J
      GO TO 31
   38 DO 39 M=1,NP
   39 C(I,M)=S(M)
      IF(NNN) 393,393,391
  391 DO 392 M=1,NNN
  392 D(I,M)=SD(M)
  393 IS=0
   40 CONTINUE
      IF(IX) 411,409,411
  407 FORMAT(15H  ((C(I,J),J=1,I3,12H),(D(J),J=1,I3, 6H),I=1,I3,15H)  AF
     1TER RERAY  )
  409 WRITE(KOUT,407) NP,NNN,N
      DO 410 I=1,N
  410 WRITE(KOUT,108)(C(I,J),J=1,NP),(D(I,J),J=1,NNN)
  411 RETURN
      END
```

REFERENCES

1. Kendall, R. M., Kelly, J. T. and Lanier, W. S., "Predictions of Premixed Laminar Flat Flame Kinetics - Including the Effects of Diffusion," Proceeding of the Stationary Source Combustion Symposium, Volume I. Fundamental Research, Environmental Protection Technology Series, EPA-600/2-76-152a, June 1976.

2. Kelly, J. T. and Kendall, R. M., "Premixed One-Dimensional Flame (PROF) Code. Development and Application", Proceedings of the Second Stationary Source Combustion Symposium, Volume IV, Fundamental Combustion Research, Interagency Energy - Environment Research and Development Program Report, EPA-600/7-77-073d, July 1977.

3. Bartlett, E. P., Kendall, R. M., and Rindal, R. A., "A Unified Approximation for Mixture Transport Properties for Multicomponent Boundary Layer Applications," Aerotherm Corporation Final Report 66-7, Part IV (also NASA CR-1063), March 14, 1967.

4. Hirschfelder, J. O., Curtiss, C. F., and Bird, R. B., Molecular Theory of Gases and Liquids, Second Printing, Corrected, with notes added, John Wiley and Sons, Inc., New York, 1964.

5. Kendall, R. M., "An Analysis of the Coupled Chemically Reacting Boundary Layer and Charring Ablator, Part V, A General Approach to the Thermochemical Solution of Mixed Equilibrium - Nonequilibrium, Homogeneous or Heterogeneous Systems," NASA CR-1064, June 1968.

6. Krieth, F., Principles of Heat Transfer, International Textbook Company, July 1968.

7. Vincenti, W. G. and Kruger, C. H., Physical Gas Dynamics, John Wiley and Sons, New York, 1965.

8. Gaydon, A. G., The Spectroscopy of Flames, Chapman and Hall, London, 1974, pp. 221-230.

9. Edwards, D. K. and Balakrishnan, A., "Thermal Radiation by Combustion Gases," Int. J. Heat and Mass Transfer, Vol. 16, 1973, pp. 221-230.

10. Sparrow, E. M. and Cess, R. D., Radiation Heat Transfer, Brooks/Cole Publishing Company, Belmont, California, 1970, pp. 218-219.

11. Hottel, H. C. and Sarofim, A. F., Radiative Transfer, McGraw-Hill Book Company, New York, 1967, pp. 229-236.

12. Mason, E. A. and Saxena, S. C., "An Approximate Formula for the Thermal Conductivity of Multicomponent Gas Mixtures," Physics of Fluid, Vol. 1, No. 5, September-October 1958, pp. 361-369.

13. Hirschfelder, J. O., "Heat Conductivity in Polyatomic, Electronically Excited, or Chemically Reacting Mixtures," Sixth Symposium (International) on Combustion, Reinhold Publishing Corp., New York, 1957, pp. 351-366.

14. Svehla, R. A., "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA TR R-132, 1962.

15. Svehla, R. A., "Thermodynamic and Transport Properties for the Hydrogen-Oxygen System," NASA SP-3011, 1964.

16. Buddenberg, J. W. and Wilke, C. R., "Calculation of Gas Mixture Viscosities," Ind. and Eng. Chem., Vol. 41, No. 7, July 1949, pp. 1345-1347.

APPENDIX A

BRIEF DEVELOPMENT AND DEMONSTRATION OF BIFURCATION APPROXIMATIONS TO DIFFUSION COEFFICIENTS

Because the development of the set of transport relations used in this code is not in the readily available combustion literature, it is appropriate to include a brief summary of the development in this report.

The formulation derives much of its utility from the simplification introduced when binary diffusion coefficients are approximated with the bifurcation relations. These are

$$D_{ij} = \frac{\overline{D}}{F_i F_j} \qquad \text{(A-1)}$$

where the F_i are diffusion factors for individual species which are independent of the system of species involved. They could be temperature dependent but this flexibility is rarely justified. The accuracy of the approximation has been tested for a variety of systems. Two examples taken from Reference 3 are shown in Tables A-1 and A-2. These results are typical when good (and consistent) sets of diffusion data are correlated. Note that these particular correlations have arbitrarily taken F_{O_2} as 1.0 to anchor an otherwise floating correlation.

In order to develop an explicit flux relationship using this approximation, it is appropriate to start with the Stefan-Maxwell relation

$$\frac{\partial x_i}{\partial s} = \sum_j \frac{x_i x_j}{\rho \mathcal{D}_{ij}} \left[\frac{j_j + D_j^T \left(\frac{\partial \ln T}{\partial s} \right)}{K_j} - \frac{j_i + D_i^T \left(\frac{\partial \ln T}{\partial s} \right)}{K_i} \right] \qquad \text{(A-2)}$$

TABLE A-1. CORRELATION OF BINARY DIFFUSION COEFFICIENTS FOR A HYDROGEN-OXYGEN SYSTEM USING PRESENT METHOD

TEMPERATURE = 12,000°R, PRESSURE = 1 ATM

Species i	j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
(a) Diffusion coefficients calculated using Lennard-Jones potential with force data from Svehla (Ref. 14)						
H	H2	36.0260	0.24713	53.1613	47.6	- 63.1
H	H2O	25.9891		23.7639	- 8.6	- 48.9
H	O	26.6238		24.7360	- 7.1	- 50.1
H	O2	22.8038		19.7757	-13.3	- 41.7
H	OH	26.4341		24.3147	- 8.0	- 49.7
H2	H2O	17.3862	0.3720	15.7877	- 9.2	- 23.5
H2	O	17.7166		16.4335	- 7.2	- 24.9
H2	O2	15.0085		13.1381	-12.5	- 11.4
H2	OH	17.5759		16.1537	- 8.1	- 24.4
H2O	O	7.0928	0.8322	7.3461	3.6	87.4
H2O	O2	5.2795		5.8730	11.2	151.6
H2O	OH	6.9078		7.2210	4.5	92.4
O	O2	5.6458	0.7995	6.1132	8.3	135.4
O	OH	7.2643		7.5163	3.5	82.9
O2	OH	5.4946	1.0000	6.0091	9.4	141.9
OH			0.8133			
Average Absolute Error					10.8	68.6
(b) Diffusion coefficients calculated using values for collision cross-sections suggested by Svehla (Ref. 15)						
H	H2	67.6000	0.2208	74.4024	10.1	- 77.1
H	H2O	28.3200		27.0030	- 4.7	- 45.4
H	O	27.7200		30.8482	11.3	- 44.3
H	O2	24.5500		22.5734	- 8.1	- 37.1
H	OH	29.5900		27.5549	- 6.9	- 47.8
H2	H2O	19.5800	0.3034	19.6568	0.4	- 21.1
H2	O	23.6000		22.4560	- 4.8	- 34.5
H2	O2	17.1900		16.4323	- 4.4	- 10.1
H2	OH	20.1600		20.0586	- 0.5	- 23.3
H2O	O	8.2950	0.8360	8.1500	- 1.7	86.3
H2O	O2	5.7150		5.9638	4.4	170.4
H2O	OH	7.1450		7.2799	1.9	116.3
O	O2	6.8500	0.7317	6.8131	- 0.5	125.6
O	OH	8.6060		8.3166	- 3.4	79.6
O2	OH	5.5520	1.0000	6.0857	9.6	178.3
OH			0.8192			
Average Absolute Error					4.8	73.1

TABLE A-2. CORRELATION OF BINARY DIFFUSION COEFFICIENTS FOR AN OXYGEN-NITROGEN-CARBON-HYGROGEN SYSTEM BASED ON DATA OF SVEHLA (Refs. 14 and 15)

TEMPERATURE = 12,000°R, PRESSURE = 1 ATM

Species i	j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
O	O2	6.8500	0.7393	6.0528	-11.6	- 4.5
O	N	7.3372		7.6554	4.3	- 10.8
O	N2	5.3995		5.6277	4.2	21.1
O	CO	5.4662		5.6846	4.0	19.7
O	CO2	4.4638		4.6277	3.7	46.5
O	C	8.0754		8.3865	3.9	- 19.0
O	C3	5.1820		5.3597	3.4	26.2
O	CN	5.3620		5.5958	4.4	22.0
O	H	27.7200		29.8130	7.6	- 76.3
O	H2	23.6000		20.4311	-13.4	- 72.2
O	H2O	8.2950		7.5057	- 9.5	- 21.1
O	OH	8.6060		7.7923	- 9.5	- 24.0
O	CH4	5.8190		6.0848	4.6	12.4
O	C2H	4.8947		5.0977	4.1	33.6
O	HCN	4.8625		5.0401	3.7	34.5
O2	N	5.6566	1.0000	5.6595	0.1	15.6
O2	N2	3.9611		4.1604	5.0	65.1
O2	CO	4.0028		4.2025	5.0	63.4
O2	CO2	3.1637		3.4212	8.1	106.7
O2	C	6.3129		6.2000	- 1.8	3.6
O2	C3	3.7100		3.9624	6.8	76.3
O2	CN	3.9623		4.1369	4.4	65.1
O2	H	24.5500		22.0402	-10.2	- 73.5
O2	H2	17.1900		15.1043	-12.1	- 62.0
O2	H2O	5.7150		5.5489	- 2.9	14.5
O2	OH	5.5520		5.7607	3.8	17.8
O2	CH4	4.4735		4.4984	0.6	46.2
O2	C2H	3.6310		3.7686	3.8	80.1
O2	HCN	3.5678		3.7260	4.4	83.3
N	N2	5.4277	0.7907	5.2620	- 3.1	20.5
N	CO	5.4763		5.3153	- 2.9	19.4
N	CO2	4.5136		4.3270	- 4.1	44.9
N	C	7.9727		7.8416	- 1.6	- 17.9
N	C3	5.2069		5.0115	- 3.8	25.6
C	CN	5.3784		5.2323	- 2.7	21.6
N	H	25.5139		27.8700	9.3	- 74.4
N	H2	17.1218		19.1036	11.6	- 61.8
N	H2O	6.9743		7.0181	0.6	- 6.2
N	OH	7.1732		7.2861	1.6	- 8.8
N	CH4	5.7836		5.6895	- 1.6	13.1
N	C2H	4.9083		4.7665	- 2.9	33.3
N	HCN	4.8645		4.7126	- 3.1	34.5

TABLE A-2. Continued

Species i	j	$\mathcal{D}_{ij}$ From Kinetic Theory (ft^2/sec) x 100	F_i	$\mathcal{D}_{ij}$ From Present Correlation (ft^2/sec) x 100	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
N2	CO	3.8943	1.0756	3.9074	0.3	68.0
N2	CO2	3.1114		3.1809	2.2	110.2
N2	C	6.0528		5.7645	- 4.8	8.1
N2	C3	3.6214		3.6840	1.7	80.6
N2	CN	3.8603		3.8463	- 0.4	69.4
N2	H	21.3750		20.4922	- 4.1	- 69.4
N2	H2	14.1671		14.0435	- 0.9	- 53.8
N2	H2O	5.0300		5.1591	2.6	30.0
N2	OH	5.2629		5.3561	1.8	24.3
N2	CH4	4.3182		4.1824	- 3.1	51.5
N2	C2H	3.5367		3.5039	- 0.9	84.9
N2	HCN	3.4655		3.4643	- 0.0	84.8
CO	CO2	3.1390	1.0647	3.2131	2.4	99.2
CO	C	6.1194		5.8229	- 4.8	9.9
CO	C3	3.6584		3.7213	1.7	72.0
CO	CN	3.8938		3.8853	- 0.2	64.8
CO	H	21.6122		20.6996	- 4.2	- 66.9
CO	H2	14.2296		14.1856	- 0.3	- 50.4
CO	H2O	5.1001		5.2113	2.2	27.1
CO	OH	5.3305		5.4103	1.5	22.3
CO	CH4	4.3595		4.2248	- 3.1	51.5
CO	C2H	3.5680		3.5394	- 0.8	80.9
CO	HCN	3.5023		3.4994	- 0.1	82.9
CO2	C	4.9902	1.3079	4.7402	- 5.0	35.0
CO2	C3	2.8753		3.0294	5.4	111.3
CO2	CN	3.1245		3.1629	1.2	102.4
CO2	H	18.4881		16.8510	- 8.9	- 59.4
CO2	H2	12.2917		11.5481	- 6.0	- 39.1
CO2	H2O	4.1217		4.2424	2.9	58.7
CO2	OH	4.3441		4.4044	1.4	50.6
CO2	CH4	3.5835		3.4393	- 4.0	82.5
CO2	C2H	2.8685		2.8813	0.4	128.0
CO2	HCN	2.7965		2.8488	1.9	133.9
C	C3	5.7767	0.7218	5.4901	- 5.0	13.2
C	CN	6.0033		5.7319	- 4.5	8.9
C	H	26.1719		30.5380	16.7	- 75.0
C	H2	18.0635		20.9280	15.9	- 63.8
C	H2O	7.5630		7.6883	1.7	- 13.5
C	OH	7.9334		7.9818	0.6	- 17.5
C	CH4	6.3330		6.2328	- 1.6	3.3
C	C2H	5.3831		5.2217	- 3.0	21.5
C	HCN	5.3406		5.1626	- 3.3	22.5

TABLE A-2. Concluded

Species i	 j	$\mathcal{D}_{ij}$ From Kinetic Theory $(ft^2/sec) \times 100$	F_i	$\mathcal{D}_{ij}$ From Present Correlation $(ft^2/sec) \times 100$	Error Using Present Correlation (Percent)	Error If All $\mathcal{D}_{ij}$ Are Assumed Equal (Percent)
C3	CN	3.6276	1.1293	3.6632	1.0	80.3
C3	H	21.0069		19.5166	- 7.1	- 68.9
C3	H2	13.9792		13.3749	- 4.3	- 53.2
C3	H2O	4.8271		4.9135	1.8	35.5
C3	OH	5.0416		5.1011	1.2	29.7
C3	CH4	4.1210		3.9833	- 3.3	58.7
C3	C2H	3.3265		3.3371	0.3	96.6
C3	HCN	3.2583		3.2994	1.3	100.7
CN	H	20.9403	1.0817	20.3763	- 2.7	- 68.8
CN	H2	13.8853		13.9641	0.6	- 52.9
CN	H2O	4.9948		5.1300	2.7	30.9
CN	OH	5.2299		5.3259	1.8	25.1
CN	CH4	4.2953		4.1588	- 3.2	52.3
CN	C2H	3.5330		3.4841	- 1.4	85.1
CN	HCN	3.4626		3.4447	- 0.5	88.9
H	H2	67.6000	0.2030	74.3967	10.1	- 90.4
H	H2O	28.3200		27.3309	- 3.5	- 76.9
H	OH	29.5900		28.3745	- 4.1	- 78.0
H	CH4	20.3467		22.1568	8.9	- 68.0
H	C2H	18.6611		18.5624	- 0.5	- 64.9
H	HCN	18.8560		18.3525	- 2.7	- 65.3
H2	H2O	19.5800	0.2963	18.7301	- 4.3	- 66.7
H2	OH	20.1600		19.4453	- 3.5	- 67.6
H2	CH4	13.7590		15.1843	10.4	- 52.4
H2	C2H	12.5045		12.7210	1.7	- 47.7
H2	HCN	12.5953		12.5771	- 0.1	- 48.1
H2O	OH	7.1450	0.8064	7.1436	- 0.0	- 8.5
H2O	CH4	5.4665		5.5782	2.0	19.6
H2O	C2H	4.5559		4.6733	2.6	43.6
H2O	HCN	4.5242		4.6205	2.1	44.6
OH	CH4	5.6987	0.7767	5.7912	1.6	14.8
OH	C2H	4.7817		4.8517	1.5	36.8
OH	HCN	4.7388		4.7969	1.2	38.0
CH4	C2H	3.9244	0.9948	3.7886	- 3.5	66.7
CH4	HCN	3.8677		3.7457	- 3.2	69.1
C2H	HCN	3.1729	1.1874	3.1381	- 1.1	106.1
HCN			1.2009			
Average Absolute Error					3.7	50.9

where x_i is the mole fraction of species i, T is the temperature, $\mathcal{D}_{ij}$ is the binary diffusion coefficient for species i and j, and D_i^T is the multicomponent thermal diffusion coefficient for species i. Substituting the approximation for binary diffusion coefficients (Eq. A-1) into the Stefan-Maxwell relation (Eq. A-2) and rewriting in terms of mass fractions, Y_i yields

$$\frac{\partial X_i}{\partial s} = \frac{\mathcal{M}^2}{\rho\bar{D}}\left(\frac{Y_i F_i}{M_i} \sum_j \frac{J_j F_j}{M_j} - \frac{F_i J_i}{M_i} \sum_j \frac{Y_i F_j}{M_j}\right) \qquad \text{(A-3)}$$

where, for convenience, a total diffusion mass flux has been defined as the sum of the molecular and thermal diffusional fluxes.

$$J_i = j_i + D_i^T \left(\frac{\partial \ \ell n \ T}{\partial s}\right) \qquad \text{(A-4)}$$

Multiplying each side of Eq. (A-3) by M_i/F_i, summing over all i, and noting that the sum of the diffusive fluxes is zero and the sum of the mass fractions is unity yields:

$$\sum_j \frac{J_j F_j}{M_j} = \frac{\rho\bar{D}}{\mathcal{M}^2} \sum_i \frac{M_i}{F_i} \frac{\partial X_i}{\partial s} \equiv \frac{\rho\bar{D}}{\mathcal{M}^2} \sum_j \frac{M_j}{F_j} \frac{\partial X_i}{\partial s} \qquad \text{(A-5)}$$

Substituting Eq. (A-5) into Eq. (A-3) results in

$$\frac{\partial X_i}{\partial s} = \frac{Y_i F_i}{M_i} \sum_j \frac{M_j}{F_j} \frac{\partial X_j}{\partial s} - \frac{\mathcal{M}^2}{\rho\bar{D}} \frac{F_i J_i}{M_i} \sum_j \frac{Y_j F_j}{M_j} \qquad \text{(A-6)}$$

At this point is is convenient to define several new quantities.

$$\mu_1 \equiv \sum_j X_j F_j \qquad \text{(A-7)}$$

$$\mu_2 \equiv \sum_j M_j X_j / F_j \qquad \text{(A-8)}$$

$$\mu_4 \equiv \sum_j (Y_i / F_j{}^2)\,(dF_j/dT) \qquad \text{(A-9)}$$

Taking the derivitor of Eq. A-8 yields

$$\frac{d\mu_2}{ds} = \sum \frac{M_j}{F_j} \frac{dX_j}{ds} = M \sum_M \frac{M_j X_j}{F_j{}^2} \frac{dF_j}{dT} \frac{dT}{ds} \qquad \text{(A-10)}$$

Introducing Equations A-7 through A-10 into A-6 yields after some rearranging

$$J_i + \frac{D_i{}^T}{T} \frac{\partial T}{\partial s} = - \frac{\rho \overline{D}}{\mu_1 F_i} \left\{ \frac{dY_i}{ds} + \frac{Y_i}{M} \left[\frac{dM}{ds} - F_i \frac{d\mu_2}{ds} - F_i M \mu_4 \frac{dT}{ds} \right] \right\} \qquad \text{(A-11)}$$

The variation of F_i with temperature as determined with a nine component system over a range from 4000° to 16000°R in Reference 3 were found to rarely exceed 0.1%. Consequently μ_4 has been taken as zero and a universal set of F_i determined for all species. Correlations of these values with molecular weight have been reasonably good as indicated in Figure A-1. The correlating equation

$$F_i = \left(\frac{M_i}{26} \right)^{0.461} \qquad \text{(A-12)}$$

is recommended when specific values of F_i are not available from other correlations. It is apparent that $\overline{D}$ must represent the temperature and pressure dependence of the $\mathcal{D}_{ij}$. Although $\overline{D}$ need have no specific relation to a real diffusion coefficient, the arbitrary choice of F_{O_2} as 1.0 prompts the interpretation of $\overline{D}$ as the self

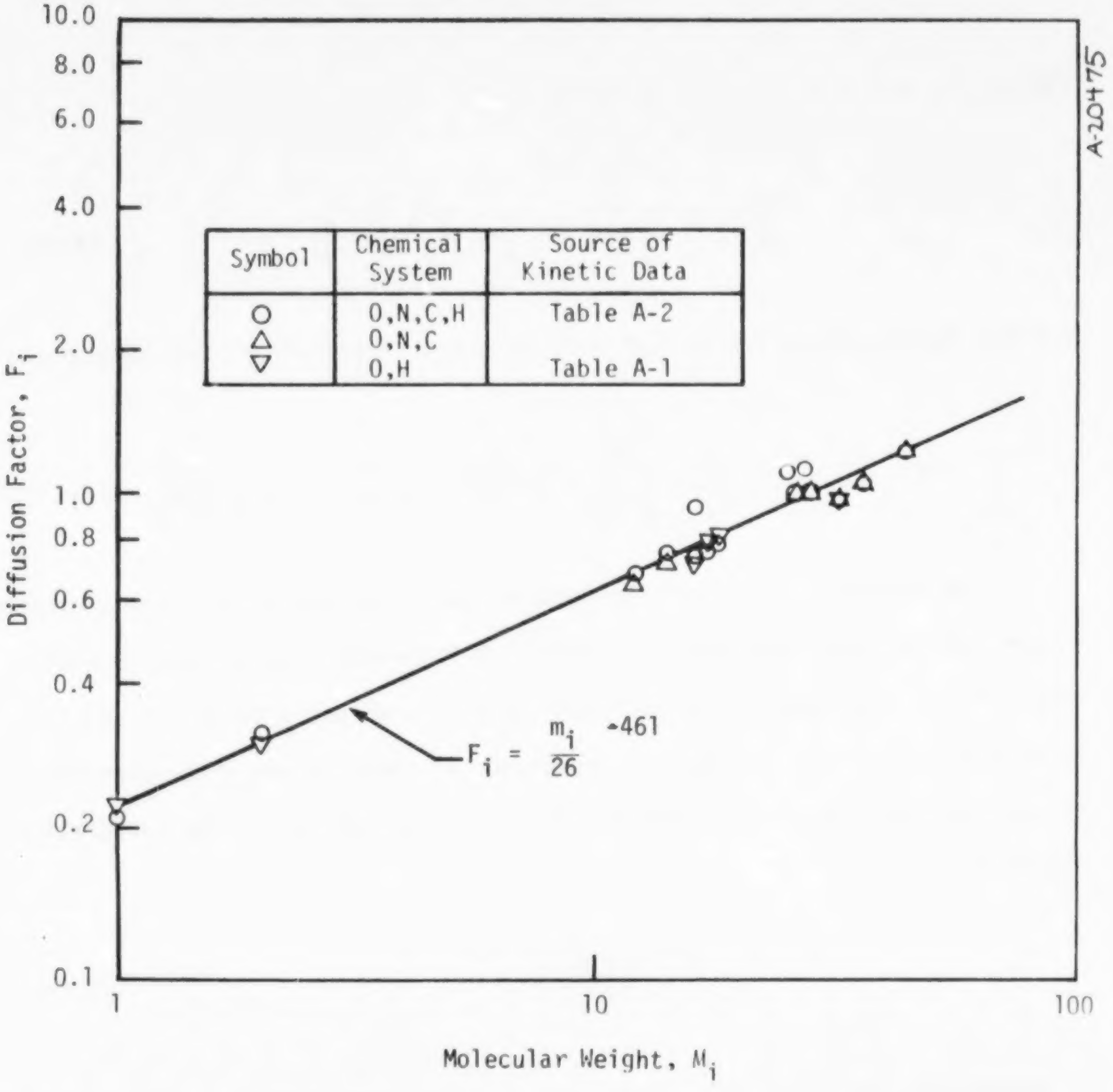

Figure A-1. Correlation of diffusion factors with molecular weight.

diffusion coefficient of O_2, $\mathcal{D}_{O_2, O_2}$. This would force a precise fit of the correlation to $\mathcal{D}_{O_2, O_2}$ but would not in general provide the best overall correlation. Ignoring this caveat we can evaluate $\mathcal{D}_{O_2, O_2}$ from the equation of Reference 4 as given by Equation 7 of the text:

$$\overline{D} = 2.628 \times 10^{-3} \frac{T(T/M_{ref})^{1/2}}{P\sigma^2_{ref}\Omega^{(1,1)*}_{ij}} \text{ (cm}^2\text{/sec)} \qquad \text{(A-13)}$$

with T in °K, P in atmospheres, and collision cross section, σ in Å. For O_2 as the reference species, σ is equal to 3.467 Å. Using the data from Reference 4, Figure A-2 demonstrates that the integral expression for transport properties is approximated by:

$$\Omega^{(1,1)*}_{ij} \approx 1.07\ [T/(\varepsilon/k)]^{-0.159}$$

where the maximum energy of attraction function, ε/k, for O_2 is 106.7 and thus:

$$\overline{D} = 0.172 \times 10^{-4}\ T^{1.659}/P \text{ (cm}^2\text{/sec)} \qquad \text{(A-14)}$$

The extension of this correlation to thermal conductivity is fully developed in the text. However, the system viscosity is also required in PROF for evaluating Reynold's number correlations. Use is made of the correlation suggested by Buddenberg and Wilke (Reference 16) and endorsed by Hirschfelder et al. (Reference 4), namely

$$\mu_{Mix} = \sum_i \frac{X_i \mu_i}{X_i + 1.385 \dfrac{RT\mu_i}{PM_i} \displaystyle\sum_{\substack{j \\ j \neq i}} \dfrac{X_j}{\mathcal{D}_{ij}}} \qquad \text{(A-15)}$$

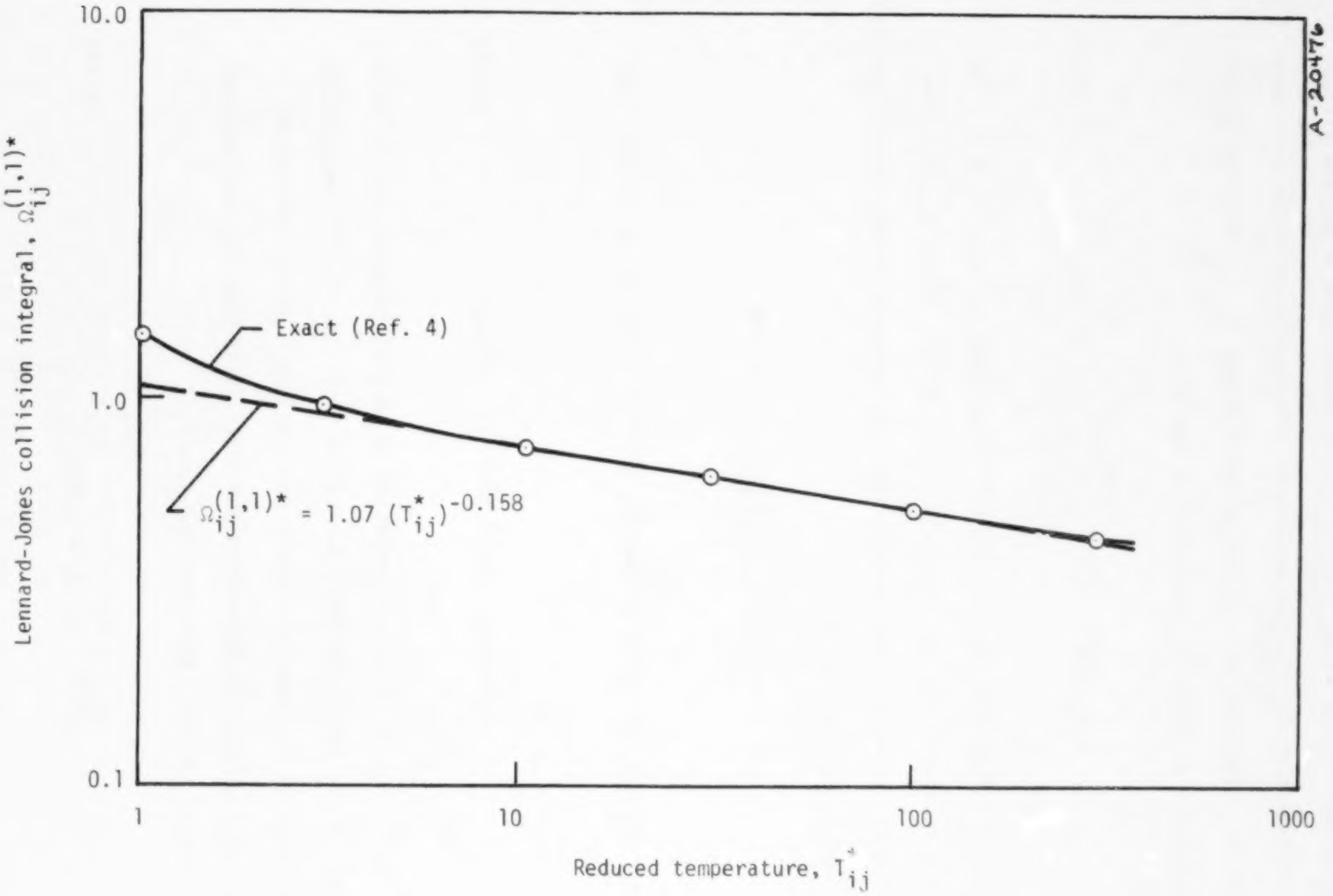

Figure A-2. Collision integral for Lennard-Jones potential.

By introducing the bifurcation relations, taking from Reference 4 the relation for pure component viscosity

$$M_i = \frac{5}{6A_{ii}^*} \rho_i \mathcal{D}_{ii}, \qquad \text{(A-16)}$$

assuming $A_{ii}^* \simeq 1.12$ (actually varies from 1.10 to 1.14 in the temperature range of interest), and adjusting 1.385 to 1.344 for simplification, there is obtained

$$\mu_{Mix} = \rho\overline{D} \frac{\mu_2}{1.344\mu_1 M} \qquad \text{(A-17)}$$

The results presented in this Appendix show that the bifurcation approximation can result in major simplification in transport property evaluations with only minimal loss in accuracy.